OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT ANALYSIS/MODEL COVER SHEET *Complete Only Applicable Items*	1. QA: QA Page: 1 of: 75

2. ☒ Analysis — Check all that apply

Type of Analysis	☐ Engineering	
	☒ Performance Assessment	
	☐ Scientific	
Intended Use of Analysis	☐ Input to Calculation	
	☐ Input to another Analysis or Model	
	☐ Input to Technical Document	
	☐ Input to other Technical Products	

Describe use:

Input to TSPA-SR analysis for waste package and drip shield degradation.

3. ☒ Model — Check all that apply

Type of Model	☐ Conceptual Model	☒ Abstraction Model
	☐ Mathematical Model	☐ System Model
	☐ Process Model	
Intended Use of Model	☐ Input to Calculation	
	☒ Input to another Model or Analysis	
	☐ Input to Technical Document	
	☒ Input to other Technical Products	

Describe use:

Input to TSPA-SR analysis for waste package and drip shield degradation

4. Title:
WAPDEG Analysis of Waste Package and Drip Shield Degradation

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-EBS-PA-000001 REV 00

6. Total Attachments:
4

7. Attachment Numbers - No. of Pages in Each:
I-17, II-16, III-35, IV-69

	Printed Name	Signature	Date
8. Originator	Joon H. Lee Kevin G. Mon Bryan E. Bullard Ahmed M. Monib	Joon Lee Kevin Mon Bryan E. Bullard Ahmed M. Monib	4/20/2000 4/20/2000 4/20/2000 4/20/2000
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11. Responsible Manager	Robert J. MacKinnon	Robert J MacKinnon	4/20/2000

12. Remarks:

Joon H. Lee is responsible for Sections 1, 2, 4, 5, 6, 7, 8, and overall technical content.
Kevin G. Mon is responsible for Sections 3, 4, 5, 6, and WAPDEG simulations.
Bryan Bullard is responsible for Sections 3, 4, 5, and Attachments I, II and III.
Ahmed Monib is responsible for Section 6, Attachment IV, and WAPDEG simulations and analysis result processing.

For TSPA-SR.

Initial Issue

Per Section 5.5.6 of AP-3.10Q, the responsible manager has determined that the subject AMR is not subject to AP-2.14Q review because the analysis does not affect a discipline or area other than the originating organization (Performance Assessment). The upstream suppliers (Waste Package Department) of inputs for this AMR have worked closely with the originator of this AMR to ensure that inputs were used properly. The downstream user of the information resulting from this AMR is the Performance Assessment (PA) Dept., which is also the originating organization of this work. Therefore, no formal AP-2.14Q reviews were requested or determined to be necessary.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET
Complete Only Applicable Items

2. Analysis or Model Title:

WAPDEG Analysis of Waste Package and Drip Shield Degradation

3. Document Identifier (including Rev. No. and Change No., if applicable):

ANL-EBS-PA-000001 REV 00

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue

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1. PURPOSE

As directed by a written development plan (CRWMS M&O 1999a), an analysis of the degradation of the drip shield and waste package in the engineered barrier system (EBS) of the Yucca Mountain repository is to be conducted. The purpose of this analysis is to assist the Performance Assessment Department (PAD) and its Engineered Barrier Performance Section in analyzing waste package and drip shield corrosion degradation as a function of exposure time under exposure conditions anticipated in the repository. This analysis will allow PAD to provide a more detailed and complete waste package and drip shield degradation abstraction and to answer the key technical issues (KTI) raised in the Nuclear Regulatory Commission (NRC) Issue Resolution Status Report (IRSR) for the Container Lifetime and Source Term (CLST) Revision 2 (NRC 1999).

The scope of the current study is limited to the nominal case, i.e., the analysis uses the best estimates of all corrosion models and simulation parameters. The WAste Package DEGradation (WAPDEG) model is the integrated model used for the analysis (CRWMS M&O 1999e). The abstractions of the process models for the corrosion degradation processes considered in this analysis and the exposure condition parameters for the waste packages and drip shields in the repository were incorporated into the WAPDEG Model. The output from the WAPDEG analysis is a set of profiles for the failure (i.e., initial breach) and subsequent number of penetration openings in the waste package and drip shield as a function of time. In the total system performance assessment (TSPA) analysis, these analysis results are used as input for waste form degradation analysis and radionuclide release analysis from failed waste packages. The WAPDEG Model is used directly in the TSPA for waste package degradation analysis. The analyses presented in this report are for the Enhanced Design Alternative II (EDA II) design that includes a drip shield placed over the waste package and backfill over the drip shield (see Design Constraint 2.2.1.1.9 of CRWMS M&O 1999g).

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this waste package and drip shield degradation analysis documentation. The Performance Assessment Operations responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation, *Conduct of Performance Assessment* (CRWMS M&O 1999b), has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (QARD) DOE/RW-0333P (DOE 2000) requirements. Preparation of this analysis did not require the classification of items in accordance with QAP-2-3, *Classification of Permanent Items.* This activity is not a field activity. Therefore, an evaluation in accordance with NLP-2-0, *Determination of Importance Evaluations* was not required.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

3.1.1 Mathcad 2000 Professional

Mathcad 2000 Professional is a commercially available software used in this analysis. This software, in accordance with AP-SI.1Q, *Software Management*, is appropriate for this application as it offers all of the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this analysis. Mathcad 2000 Professional was executed on a DELL PowerEdge 2200 Workstation equipped with two Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system.

3.1.2 Excel 97 SR-2

Excel 97 SR-2 is a commercially available software used in this analysis. This software, in accordance with AP-SI.1Q, *Software Management*, is appropriate for this application as it offers all of the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this calculation. Excel 97 SR-2 was executed on a DELL PowerEdge 2200 Workstation equipped with two Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system.

3.1.3 WAPDEG 4.0

The WAPDEG software was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the models documented in this analysis. The WAPDEG software is currently unqualified and is used in this analyses and models report in accordance with Section 5.11 of AP-SI.1Q, Rev. 2, ICN 4. The following information is used to identify the WAPDEG software:

Software Name: WAPDEG

Software Version: 4.0

STN: 10000-4.0-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The WAPDEG simulations were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system.

WAPDEG version 4.0 is, in accordance with AP-SI.1Q, *Software Management*, an appropriate tool for this application, because it was specifically designed to calculate drip shield and waste package failure profiles in a manner consistent with the information requirements of the total system performance assessment model. The software was used within its intended range of validation (CRWMS M&O 1999d).

3.1.4 GVP 1.01

Software routine Gaussian Variance Partitioning (GVP) was also developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the variance sharing of stochastic model parameters. This software is appropriate for this application as it was developed to implement the results of the analyses. Details of the software routine verification are presented in Attachment I. The GVP software routine is typically compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0D, Standard Edition. The GVP software routine is identified as follows:

Name and Version Number: GVP version 1.01

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

3.1.5 MFD 1.01

Software routine ManuFacturing Defects (MFD) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the probability of the occurrence and size of manufacturing defects in the closure-lid welds of the waste package outer barrier. This software is appropriate for this application as it was developed to implement the results of the analyses. Details of the software routine verification are presented in Attachment II. The MFD software routine is typically compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0D, Standard Edition. The MFD software routine is identified as follows:

Name and Version Number: MFD version 1.01

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

3.1.6 SCCD 1.01

Software routine Stress Corrosion Cracking Dissolution (SCCD) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the stress and stress intensity factor profiles in the closure-lid welds of the waste package outer barrier. This software is appropriate for this application as it was developed to implement the results of the analyses. Details of the software routine verification are presented in Attachment III. The SCCD software routine is typically compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0D, Standard Edition. The SCCD software routine is identified as follows:

Name and Version Number: SCCD version 1.01

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

3.1.7 PREWAP 1.0

Software routine PREWAP was also developed, in accordance with AP-SI.1Q, *Software Management*, to extract the data for the time-history of temperature and relative humidity of drip shields and waste packages, and pH of water contacting the drip shields and waste packages from various source tables. The extracted data are prepared as an output table in a format that is used as input to the WAPDEG code. The PREWAP routine is a stand alone executable that does not operate as a DLL under (TSPA-SR) software. This allows the WAPDEG input to be prepared independent of (TSPA-SR) software reducing run time for TSPA SR realizations. This software is appropriate for this application as it was developed to implement the results of the analyses. The PREWAP software routine interpolates thermophysical properties (i.e., pH and chloride ion concentration) as a function of repository exposure conditions (such as temperature and relative humidity). The thermophysical property input tables used for the PREWAP software do not cover the entire space of repository exposure conditions over which they are used. The PREWAP software routine uses bounding values when this situation is encountered. The use of bounding values has no impact on the results of this AMR because no models used in this analysis are chemistry dependent, with the exception of the localized corrosion initiation model used for the Alloy 22 waste package outer barrier (see Sections 4.1.5 and 6.3.10), which uses exposure pH. However, the localized corrosion initiation model used for the Alloy 22 waste package outer barrier does not allow for localized corrosion initation at any pH (based on the $\pm 4\sigma$ confidence interval, see Figure 1). Therefore, the use of bounding values in the PREWAP software routine has no impact on the results of this AMR. Details of the software routine verification are presented in Attachment IV. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 6.0A, Professional Edition. The PREWAP software routine is identified as follows:

Name and Version Number: PREWAP version 1.0

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

3.1.8 GoldSim 6.02.006

The GoldSim software (Golder Associates 2000) is used to implement the total system performance assessment model. The software was used to run the WAPDEG Model and implement other component models that are documented in this analysis. The GoldSim software was used to pass input to the WAPDEG software. The following information is used to identify the GoldSim software:

Software Name: GoldSim

Software Version: 6.02.006

STN: 10286-6.02.006-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The GoldSim software was executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system.

GoldSim version 6.02 is an appropriate tool for this application, because it was specifically designed to call WAPDEG 4.0. The GoldSim code was used within the range of values for which it was validated.

3.2 MODELS USED

The WAPDEG Model is documented in this report. The WAPDEG Model is composed of the WAPDEG code (see Section 3.1.3) and a number of sub-models (abstractions of process level models), which are implemented within the WAPDEG code. In this Section, these submodels are discussed. The DTNs, statements of appropriateness for intended use, etc. made for each of these submodels constitute documentation of the WAPDEG Model which they comprise. The WAPDEG Model integrates the sub-models for waste package and drip shield degradation with expected repository exposure parameters to yield waste package and drip shield degradation profiles appropriate for use in assessing the proposed repository at Yucca Mountain. Degradation profiles consist of time histories of the first failure (initial breach) times and the number and type (pit, crack, patch) of penetrations versus time for both the waste package and drip shield. The WAPDEG Model is appropriate for its intended use as it was specifically designed to develop waste package and drip shield degradation profiles for use in assessing the proposed repository at Yucca Mountain. This WAPDEG Model makes use of the WAPDEG software within its intended range of validation (CRWMS M&O 1999d).

3.2.1 Drip Shield General Corrosion Model

This model is discussed in Sections 4.1.3 and 6.3.5. Details of the general corrosion rate distribution used for the Titanium grade 7 drip shield (WDgTi7Sr00.cdf) are given in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003.

This model is implemented within the WAPDEG software (see Section 3.1.3) and is appropriate for its intended use because it was specifically developed for modeling general corrosion degradation of the Titanium grade 7 drip shield. This model was used within its range of validation (see Section 6.3.5).

3.2.2 Waste Package Outer Barrier General Corrosion Model

This model is discussed in Sections 4.1.4 and 6.3.6. Details of the primary general corrosion rate distribution used for the Alloy 22 waste package outer barrier (WDgA22SR00.cdf) are given in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003.

This model is implemented within the WAPDEG software (see Section 3.1.3) and is appropriate for its intended use, because it was specifically developed for modeling general corrosion degradation of the Alloy 22 waste package outer barrier. This model was used within its range of validation (see Section 6.3.6).

3.2.3 Relative Humidity Abstraction Model

This model is discussed in Sections 4.1.2 and 6.3.8. The relationship between the critical threshold RH and exposure temperature is based on the assumption of the presence of a sodium nitrate ($NaNO_3$) salt film on the waste package and drip shield surface and the deliquescence point of the salt as documented in the Analyses and Models Report entitled *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000b, Tables 7 and 8) (also see DTN: LL991212305924.108). The relationship between the critical threshold RH and exposure temperature is given by a lookup table.

This model is implemented within the WAPDEG software (see Section 3.1.3) and is appropriate for its intended use, because it was specifically developed for modeling the criterion for initiation of corrosion degradation of the Alloy 22 waste package outer barrier and Titanium grade 7 drip shield. This model was used within its range of validation (see Section 6.3.8).

3.2.4 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

This model is discussed in Sections 4.1.5 and 6.3.10. The localized corrosion initiation model used for the Alloy 22 waste package outer barrier is validated in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d) (DTN: MO0003SPAPCC03.004).

This model is implemented within the WAPDEG software (see Section 3.1.3) and is appropriate for its intended use because it was specifically developed for modeling the criterion for localized corrosion initiation and rate of propagation on the Alloy 22 waste package outer barrier. The localized corrosion initiation portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model was used within its range of validation (see CRWMS M&O 2000d and Sections 4.1.5 and 6.3.10). However, as discussed in Section 3.1.7, the PREWAP subroutine does make use of bounding pH values in the preparation of the input for the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model. The localized corrosion rate portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model is validated by the observation, in Section 5.4, that the localized corrosion rate data is a conservative representation of localized corrosion rate of Alloy 22. This observation provides confidence in the adequacy of the localized corrosion rate model and that it is appropriate for its intended use.

3.2.5 Manufacturing Defect Abstraction Model

This model is discussed in Sections 4.1.7 and 6.3.11. All of the data and parameters used in this model are documented in the calculation entitled *Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis* (CRWMS M&O 2000g) and are tracked by DTN: MO0001SPASUP03.001.

This model is implemented partly within the WAPDEG software (see Section 3.1.3) and partly within the MFD software routine (see Attachment II). The Manufacturing Defect Abstraction Model is validated in Section 6.3.11. The Manufacturing Defect Abstraction Model was used within its range of validation. The Manufacturing Defect Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the occurrence of manufacturing defects in the Alloy 22 waste package outer and inner lid weld regions.

3.2.6 Stress and Stress Intensity Profile Abstraction Model

This model is discussed in Sections 4.1.8 and 6.3.12. All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003.

This model is implemented partly within the WAPDEG software (see Section 3.1.3) and partly within the SCCD software routine (see Attachment III). The Stress and Stress Intensity Profile Abstraction Model is validated in Section 6.3.12. The Stress and Stress Intensity Profile Abstraction Model was used within its range of validation. The Stress and Stress Intensity Profile Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the stress and stress intensity profiles in the Alloy 22 waste package outer and inner lid weld regions.

3.2.7 Slip Dissolution Abstraction Model

This model is discussed in Sections 4.1.9 and 6.3.13. All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003.

This model is implemented partly within the WAPDEG software (see Section 3.1.3) and partly within the SCCD software routine (see Attachment III). The Slip Dissolution Abstraction Model is validated in Section 6.3.13. The Slip Dissolution Abstraction Model was used within its range of validation. The Slip Dissolution Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the slip dissolution stress corrosion cracking process in the Alloy 22 waste package outer and inner lid weld regions.

3.2.8 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model

This model is discussed in Sections 4.1.10 and 6.3.14. All of the parameters used in this model are documented in the AMR entitled *General and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.9 paragraph 1). General corrosion rates will be enhanced by a uniformly distributed factor with a lower bound of 1 and an upper bound of 2, above 90% relative humidity.

This model is implemented within the WAPDEG software (see Section 3.1.3). The Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model is validated in Section 6.3.14. The Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model was used within its range of validation. The Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the MIC on the Alloy 22 waste package outer barrier.

3.2.9 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model

This model is discussed in Sections 4.1.11 and 6.3.15. All of the parameters used in this model are documented in the AMR entitled *General and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.7.3 paragraph 2). General corrosion rates of the waste package outer barrier are enhanced by a factor uniformly distributed between 1 and 2.5 (i.e., no enhancement up to the general corrosion rate being multiplied by 2.5) (CRWMS M&O 2000e, Section 6.7.3 paragraph 2).

This model is implemented within the WAPDEG software (see Section 3.1.3). The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model is validated in Section 6.3.15. The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model was used within its range of validation. The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the effect of aging and phase instability on the Alloy 22 waste package outer barrier.

4. INPUTS

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur, as a result of completing the confirmation activities, will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

4.1 DATA AND PARAMETERS

4.1.1 Waste Package and Drip Shield Design Input

Waste package and drip shield dimensions were obtained and are presented in Table 1.

Table 1. Waste Package and Drip Shield Dimensions.

Parameter Name	Parameter Value	Source
Waste Package Outer Shell Extension (“Skirt”) ID	1564 mm	CRWMS M&O 1999c Item 2 page 1 of 1
Waste Package Outer Shell Length	4775 mm	CRWMS M&O 1999c Item 2 page 1 of 1
Waste Package Outer Shell Thickness	20 mm	CRWMS M&O 1999c Item 2 page 1 of 1
Drip Shield Height	2521 mm	CRWMS M&O 2000a Page 4 of 5
Drip Shield Width	2512 mm	CRWMS M&O 2000a Page 4 of 5
Drip Shield Thickness	15 mm	CRWMS M&O 2000a Page 4 of 5

Note: The waste package outer shell skirt ID is approximately equal to the waste package outer barrier outer diameter (CRWMS M&O 1999c, Item 2 page 1 of 1).

Note: The waste package outer shell length is mislabeled as “Inner Shell” in CRWMS M&O 1999c.

These inputs are used to calculate the total surface areas of the waste package barriers or drip shield. This data is preliminary and was transmitted in accordance with AP-3.14Q, *Transmittal Of Input.* These surface areas are discussed further in Section 5.1.

4.1.2 Relative Humidity Threshold Abstraction Model

The critical relative humidity (RH) threshold for the initiation of corrosion degradation (general corrosion, localized corrosion and stress corrosion cracking processes) is a function of exposure temperature. The relationship between the critical threshold RH and exposure temperature is based on the assumption (Section 5.2) of the presence of a sodium nitrate ($NaNO_3$) salt film on the waste package and drip shield surface and the deliquescence point of the salt as documented in the Analyses and Models Report entitled *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000b, Tables 7 and 8) (also see Data Tracking Number (DTN): LL991212305924.108). This data is considered accepted data.

4.1.3 Drip Shield General Corrosion Abstraction Model

Details of the general corrosion rate distribution used for the Titanium grade 7 drip shield (WDgTi7Sr00.cdf) are given in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003. This data is qualified but does require verification. Also see Section 6.3.5 for discussion of implementation.

4.1.4 Waste Package Outer Barrier General Corrosion Abstraction Model

Details of the primary general corrosion rate distribution used for the Alloy 22 waste package outer barrier (WDgA22SR00.cdf) are given in a calculation entitled *Calculation of General*

Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003. This data is qualified. Also see Section 6.3.6 for discussion of implementation.

4.1.5 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

The localized corrosion initiation model used for the Alloy 22 waste package outer barrier and associated model parameters are discussed in the Analysis Model Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d). In summary, the localized corrosion initiation threshold is based on potentiodynamic polarization data for Alloy 22 measured in several repository-relevant solution compositions. The data consisted of measurements of the critical potential for localized corrosion initiation, *Ecrit1*, and the corrosion potential, *Ecorr*, at various temperatures, chloride concentrations and *pH* values. The potential difference $\Delta E = (Ecrit1 - Ecorr)$ (in mV) was fit to a function of *pH* (the dependence of the potential difference on temperature and chloride concentration was negligible)

$$DE = c_0 + c_1 \cdot pH + c_2 \cdot pH^2 + e \qquad \text{(Eq. 1)}$$

where c_o, c_1, and c_2 are constants determined from fitting to Equation 1 to the collected potential difference data. e (referred to as the "error" variance or "residual" variance) is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero. Linear regression gives the following estimates for the parameters in Equation 3: $c_o = 1160$, $c_1 = -193$ and $c_2 = 12.0$. The covariance matrix (s) and correlation matrix (C) resulting from the fitting procedure were determined to be:

$$s = \begin{bmatrix} 3530 & -1040 & 64.4 \\ -1040 & 364 & -24.4 \\ 64.4 & -24.4 & 1.69 \end{bmatrix} \quad C = \begin{bmatrix} 1 & -0.915 & 0.835 \\ -0.915 & 1 & -0.982 \\ 0.835 & -0.982 & 1 \end{bmatrix} \qquad \text{(Eq. 2)}$$

and the variance of e determined from the linear regression fitting procedure is *4670.*

Figure 1 shows a plot of how the median potential difference (ΔE) given by Equation 1 varies with *pH.* Also shown are the $\pm 3\sigma$ and $\pm 4\sigma$ confidence intervals. These inputs are tracked by DTN: MO0003SPAPCC03.004 and are qualified.

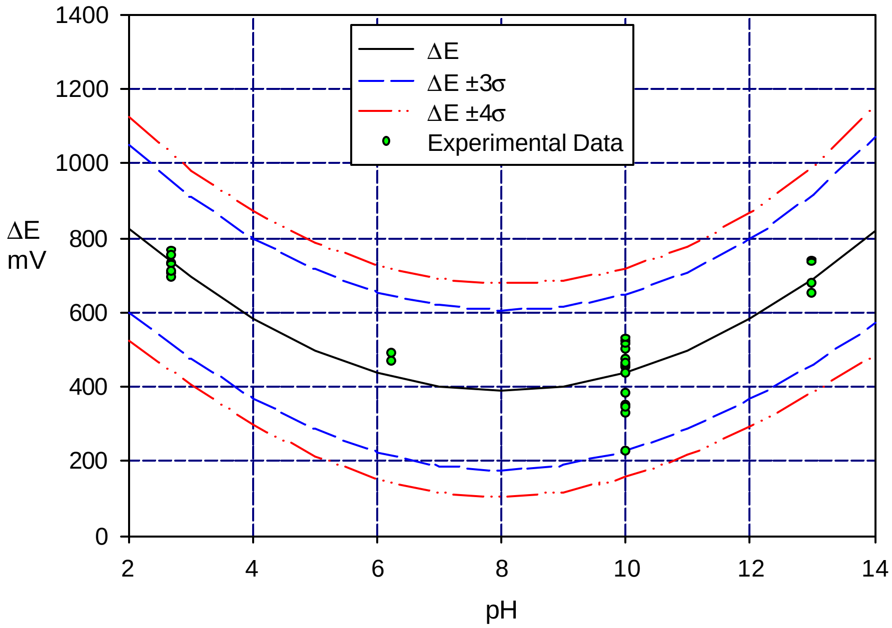

Figure 1. Plot of ΔE vs. *pH* for Alloy 22 from Equation 1 and 2 showing the $\pm 3\sigma$ and $\pm 4\sigma$ confidence intervals and the experimental data from which the model was derived.

The distribution of localized corrosion rates presented in Table 22 of the AMR entitled *General and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.6.6) will be used for localized corrosion modeling of the Alloy 22 waste package outer barrier. These rates are reproduced in Table 2 (with rates converted from μm/yr to mm/yr). The localized corrosion rates are assumed to be loguniformly distributed (see Section 5.4).

Table 2. Distribution of Localized Corrosion Rates for Alloy 22 (DTN: LL991213705924.109).

Percentile (%)	Localized Corrosion Rate (mm/yr)
0^{th}	12.7E-3
50^{th}	127E-3
100^{th}	1270E-3

These data are tracked by DTN: LL991213705924.109 and are unqualified, however, these data are considered to be conservative bounding values to the Alloy 22 localized corrosion rates (see Section 5.4) and thus are considered verified.

4.1.6 Drip Shield Localized Corrosion Initiation Threshold and Rate Abstraction Models

The localized corrosion initiation model used for the titanium grade 7 drip shield and model parameters are discussed in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS

M&O 2000d). In summary, the localized corrosion initiation threshold is based on potentiodynamic polarization data for titanium grade 7 measured in several repository-relevant solution compositions. The data consisted of measurements of the critical potential for localized corrosion initiation, *Ecrit1*, and the corrosion potential, *Ecorr*, at various temperatures, chloride concentrations and *pH* values. The potential difference *DE* = (*Ecrit1 – Ecorr)* (in mV) was fit to a function of *pH* (the dependence of the potential difference on temperature and chloride concentration was negligible).

$$DE = f_0 + f_1 \cdot pH + e \qquad \text{(Eq. 3)}$$

where f_o, and f_1 are constants determined from fitting to Equation 3 to the collected potential difference data. ***e*** (referred to as the "error" variance or "residual" variance) is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero. Linear regression gives the following estimates for the parameters in Equation 3: $f_o = 1670$ and $f_1 = 52.2$. The covariance matrix (*s*) and correlation matrix (*C*) resulting from the fitting procedure were determined to be:

$$s = \begin{bmatrix} 2040 & -230 \\ -230 & 31.9 \end{bmatrix} \quad C = \begin{bmatrix} 1 & -0.904 \\ -0.904 & 1 \end{bmatrix} \qquad \text{(Eq. 4)}$$

and the variance of ***e*** determined from the linear regression fitting procedure is *1080.*

Figure 2 shows a plot of how the median potential difference (*DE*) given by Equation 3 varies with *pH.* Also shown are the ±3σ and ±4σ confidence intervals. These inputs are tracked by DTN: MO0003SPAPCC03.004 and are qualified.

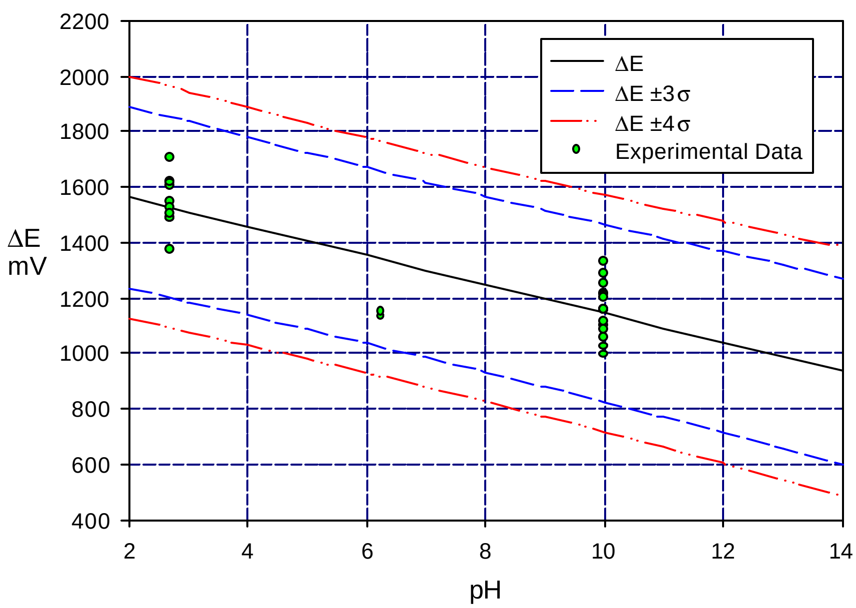

Figure 2. Plot of *DE* vs. *pH* for titanium grade 7 from Equation 3 and 4 showing the ±3σ and ±4σ confidence intervals and the experimental data from which the model was derived.

The distribution of localized corrosion rates presented in Table 16 of the AMR entitled *General and Localized Corrosion of the Drip Shield* (CRWMS M&O 2000f, Section 6.7) will be used for localized corrosion modeling of the titanium grade 7 drip shield. These rates are reproduced in Table 3 (with rates converted from μm/yr to mm/yr).

Table 3. Distribution of Localized Corrosion Rates for Titanium grade 7.

Percentile (%)	Localized Corrosion Rate (mm/yr)
0th	490E-3
100th	1120E-3

The localized corrosion rates are uniformly (or rectanglularly) distributed between the bounds specified in Table 3 (CRWMS M&O 2000f, Section 6.7, paragraph 4). These data are tracked by DTN: LL981212005924.062 and are unqualified, however, these data are considered to be conservative bounding values to the Titanium grade 7 localized corrosion rates (see Section 5.3) and thus are considered verified.

4.1.7 Manufacturing Defect Abstraction Model (Waste Package Closure-Lid Welds)

Table 4 lists the inputs to the manufacturing defects abstraction analysis for the waste package outer barrier closure-lid welds.

Table 4. Stress and Stress Intensity Profile Data and Parameters and Their Sources

Parameter Name	Parameter Value	Source
Lid Thickness	25 mm Alloy 22 for Outer Lid 10 mm Alloy 22 for Inner Lid	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
Lid Radius	0.76 m for Both lids	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
b, Location Parameter for Probability of Non-Detection	Uniform over the range (1.6, 5.0) mm	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
, the scale parameter of the non-detection probability	Uniform over the range (1, 3)	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
y, the fraction of surface breaking fractures	Uniform over the range (0.0013, 0.0049)	CRWMS M&O 2000g DTN: MO0001SPASUP03.001

All of the data and parameters discussed in this section were documented in the calculation entitled *Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis* (CRWMS M&O 2000g) and are tracked by DTN: MO0001SPASUP03.001 and are unqualified preliminary data.

4.1.8 Stress and Stress Intensity Profile Abstraction Model (Waste Package Closure-Lid Welds)

Data and parameters that are input to this analysis include stress and stress intensity profiles (stress or stress intensity versus depth) and model parameters appropriate for both the outer and inner closure-lids of the waste package outer barrier. Table 5 summarizes these data, their sources, data tracking numbers (DTNs), and Table numbers. These data are considered unqualified preliminary data.

Table 5. Stress and Stress Intensity Profile Data and Parameters and Their Sources

Parameter Name	Parameter Value	Source
Stress Intensity Factor Profiles	Table 6	CRWMS M&O 2000i MO0004SPASDA04.003
Stress Profile Coefficients	Table 7	CRWMS M&O 2000i MO0004SPASDA04.003
Yield Strength	Table 8	CRWMS M&O 2000i MO0004SPASDA04.003
Fraction of Yield Strength	Table 8	CRWMS M&O 2000i MO0004SPASDA04.003

Table 6. Stress intensity factor (K_I) vs. depth tables for the outer and inner closure-lids of waste package outer barrier.

Outer Lid		Inner Lid	
KI (MPa*m½)	Depth (mm)	KI (MPa*m½)	Depth (mm)
-8.096912553	0.3988	-7.201806034	0.3277
-11.08864448	0.8001	-10.05117186	0.6579
-13.12743778	1.1989	-12.14661052	0.9855
-14.62395207	1.6002	-13.83718048	1.3132
-15.74125563	1.9990	-15.26051182	1.6408
-16.56494834	2.4003	-16.48813922	1.971
-17.16634511	2.7991	-17.60873931	2.2987
-17.5702798	3.2004	-18.62418012	2.6264
-17.79521296	3.5992	-19.34568044	2.954
-17.85960516	3.9980	-18.27353932	3.2842
-17.77785124	4.3993	-17.05876838	3.6119
-17.56148906	4.7981	-15.73543176	3.9395
-17.22755067	5.1994	-14.40693057	4.2697
-16.78515648	5.5982	-13.09502192	4.5974
-16.23441637	5.9995	-11.74410433	4.9251
-15.58159374	6.3983	-10.37129779	5.2527
-14.83251247	6.7970	-8.992063026	5.5829
-13.99233711	7.1984	-7.619959749	5.9106
-13.06249616	7.5971	-6.28349195	6.2382
-12.03771518	7.9985	-5.021547684	6.5659
-10.93137807	8.3972	-3.791766552	6.8961
-9.747286832	8.7986	-2.602642611	7.2238
-8.489320377	9.1973	-1.461856773	7.5514
-7.161148843	9.5987	-0.376262524	7.8791
-5.7664094	9.9974	0.6479086	8.2093
-4.327309665	10.3962	1.602739435	8.5369
-2.830795383	10.7975	2.489890331	8.8646
-1.280437794	11.1963	3.304704392	9.1948
0.320255595	11.5976	4.043027992	9.5225
1.967753102	11.9964	4.701256926	9.8501
3.658542826	12.3977	5.276226526	10.1778
5.415098304	12.7965	5.809253288	10.508
7.218783158	13.1978	6.267459831	10.8356
9.05768593	13.5966	6.633989902	11.1633
10.92825736	13.9954	6.907239191	11.491
12.82690422	14.3967	7.086141819	11.8212
14.74987947	14.7955	7.170016506	12.1488

Outer Lid		Inner Lid	
KI (MPa*m½)	Depth (mm)	KI (MPa*m½)	Depth (mm)
16.73175271	15.1968	7.171796631	12.4765
18.7698867	15.5956	7.082153019	12.8067
20.82285508	15.9969	6.8851964	13.1343
22.88648224	16.3957	6.581695963	13.462
24.95692222	16.7945	6.173014275	13.7897
27.03021919	17.1958	5.661052333	14.1199
29.13461342	17.5946	5.214086954	14.4475
31.33328838	17.9959	5.185517036	14.7752
33.52559005	18.3947	5.092620849	15.1028
35.70701317	18.7960	4.940639873	15.433
37.87294261	19.1948	4.735255128	15.7607
40.01865333	19.5961	4.482741007	16.0884
42.13953021	19.9949	4.18995429	16.4186

Stress (σ_s in MPa) as a function of depth (x in mm) is given by a third order polynomial equation of the form (CRWMS M&O 2000h, Section 6.2.2.5):

$$\sigma_s(x) = A_0 + A_1 \cdot x + A_2 \cdot x^2 + A_3 \cdot x^3 \quad \text{(Eq. 5)}$$

where the values of the coefficients (A_i's) are given in Table 7.

Table 7. Stress Coefficients used for the outer and inner closure-lids of waste package outer barrier in metric units (i.e., stress in MPa).

Coefficient	Outer Lid	Inner Lid
A_0	-356.26778	-437.720543
A_1	37.180767	176.967239
A_2	1.436391	-15.606072
A_3	-0.065282	0.367099

The provided hoop stress state was determined to vary with angle (θ) around the circumference of the waste package closure-lid welds ($\theta = 0$ point arbitrarily chosen) according to the following functional form (CRWMS M&O 2000h, Section 6.2.2.5):

$$\sigma_t(x,\theta) = \sigma_s(x) - (17.236892) \cdot (1 - \cos(\theta)) \quad \text{(Eq. 6)}$$

Note that σ_s (defined in Equation 5) uses the stress coefficients (A_i) defined in Table 7 with x in units of mm. Based on the angular stress variation in Equation 6, the stress intensity variation with angle is given by (CRWMS M&O 2000h, Section 6.2.2.5):

$$K_t(x,\theta) = K_I(x) \cdot \left(\frac{\sigma_t(Thck,\theta)}{\sigma_t(Thck,0)} \right) \quad \text{(Eq. 7)}$$

where $Thck$ is the lid thickness and $K_I(x)$ is given by the values in Table 6. The uncertainty in the stress state and stress intensity factor is introduced through a scaling factor, $rscale(\ ,z)$, where z represents the number of standard deviations away from the median value. The scaling factor is also a function of the yield strength (*YS*) and yield strength scaling factor (*F*). The yield strength and yield strength scaling factor used for the two lids are given in Table 8.

Table 8. Yield Strength and Fraction of Yield Strength for the Outer and Inner Closure-Lids of Waste Package Outer Barrier.

	Outer Lid	Inner Lid
Yield Strength (*YS*)	322.3 MPa	322.3 MPa
Yield Strength Scaling Factor (*F*)	0.05	0.05

The functional form of the scaling factor, *rscale*(θ,*z*) (CRWMS M&O 2000h, Section 6.2.2.5), is shown in Equation 8.

$$rscale(\theta, z) = \frac{\sigma_t(Thck, \theta) + z \cdot \left(\frac{YS \cdot F}{3} \right)}{\sigma_t(Thck, \theta)} \qquad \text{(Eq. 8)}$$

The elicited radial crack path for the outer lid (driven by the hoop stress) is in a direction normal to the outer surface (CRWMS M&O 2000h), thus, the crack length corresponds to the crack depth for the outer lid. However, the elicited crack path for the inner lid is at an angle to the normal of the lid surface (CRWMS M&O 2000h, p. A-60 and A-61), and the depth of the crack with respect to the surface is determined by projecting the crack length onto the lid surface normal. The angle of projection (37.5 degrees) was estimated from the length of the hoop stress plane and the thickness of the inner lid (see CRWMS M&O 2000h, Figure AI-1). Thus the *sine* of the angle multiplied by the crack length results in the crack depth with respect to the inner lid surface (i.e., in a direction normal to the inner lid outer surface).

All of the data and parameters discussed in this section were documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003 and are unqualified preliminary data.

4.1.9 Slip Dissolution Abstraction Model

The Slip Dissolution Model for stress corrosion cracking requires a threshold stress, an incipient crack density, and crack growth rate model parameters. These data and their sources are listed in Table 9.

Table 9. Slip Dissolution Model Parameters and Their Sources

Parameter Name	Parameter Value	Source
Threshold Stress	Uniform over the range (0.2, 0.3) fraction of the Yield Strength	CRWMS M&O 2000i MO0004SPASDA04.003
Incipient crack size	0.05 mm	CRWMS M&O 2000i MO0004SPASDA04.003
n, crack growth exponent	Uniform over the range (0.75, 0.84)	CRWMS M&O 2000i MO0004SPASDA04.003
A, crack growth preexponent	Equation 9	CRWMS M&O 2000i MO0004SPASDA04.003

The threshold stress is defined as the minimum stress at which cracks start growing at a rate determined by Equation 9. As suggested in the upstream process model analysis (CRWMS M&O 2000h, Section 6.5.2), the threshold stress can range from 20 to 30 percent of the yield strength (see Table 8) and the range of variation is due to uncertainty only. Furthermore, the uncertainty range is given by a uniform distribution. Thus, the resulting uncertainty range for the threshold stress is uniformly distributed between 64.46 and 96.60 MPa. In the Stress Corrosion Cracking (SCC) analysis of waste package closure-lid weld with WAPDEG, for each realization (or each run), the threshold stress is sampled from the range with a uniform distribution, and the sampled threshold stress is used for all the closure-lid weld patches of the waste packages under consideration.

In the SCC process, the crack initiation is associated with microscopic crack formation at localized corrosion or mechanical defect sites that are associated with pitting, intergranular attack, scratches, weld defects, or design notches. The crack growth rate increases as the microscopic cracks coalesce, and approaches a steady-state value when a crack can be detected (CRWMS M&O 2000h, Section 6.4.1). The current analysis assumes that the above crack depth range represents the minimum crack depth for which the slip dissolution model can be applied. Those cracks are referred to as "incipient" cracks. An exponential distribution with a maximum size of 50 µm and a median size of 20 µm was suggested for the incipient crack size distribution. Because the effect of differing incipient crack sizes (within the suggested range) on crack penetration time is much smaller than the other model parameters (i.e., n and K_I in Equation 9), the maximum crack size (50 µm or 0.05 mm) is used for all the incipient cracks considered in the SCC analysis, a conservative assumption (see Section 5.7).

Once crack growth initiates the crack(s) grow at a velocity given by (CRWMS M&O 2000h, Section 6.4.4):

$$V_t = \overline{A}\left(K_I\right)^{\overline{n}} \qquad \text{(Eq. 9)}$$

where V_t is the crack growth rate in mm/s, and K_I is the stress intensity factor in MPa(m)$^{1/2}$. Parameters, $\overline{A}$ and $\overline{n}$, in the above equation are expressed as follows.

$$\overline{A} = 7.8x10^{-2}\, n^{3.6}\left(4.1x10^{-14}\right)^{n} 3.1558149x10^{7} \qquad \text{(Eq. 10)}$$

$$\bar{n} = 4n \quad \text{(Eq. 11)}$$

Note that 3.1558149E+7 is a conversion factor between seconds and years.

CRWMS M&O 2000h (Section 6.4.4) indicates that the uncertainty in the model parameter n is represented by a uniform distribution with an upper bound of 0.84 and a lower bound of 0.75, and thus $\bar{n}$ would be represented by a uniform distribution with an upper bound of 3.36 and a lower bound of 3.

All of the data and parameters discussed in this section were documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003 and are unqualified preliminary data.

4.1.10 Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model

The Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Model requires a threshold relative humidity for microbial activity and a general corrosion rate multiplier to model the affect of microbial activity. These data and their sources are listed in Table 10.

Table 10. Waste Package Outer Barrier Microbial Induced Corrosion Model Parameters and Their Sources

Parameter Name	Parameter Value	Source
Threshold RH	0.9	CRWMS M&O 2000e Section 6.10
General Corrosion Multiplier Distribution	Uniform over the range (1, 2)	CRWMS M&O 2000e Section 6.8

According to the upstream analysis entitled *General and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.10 paragraph 1), general corrosion rates will be enhanced to model the effect of MIC above 90% relative humidity. The upstream analysis goes on to recommend the general corrosion rate of the waste package outer barrier be enhanced by a factor between 1 and 2 (i.e., no enhancement up to the general corrosion rate being doubled) (CRWMS M&O 2000e, Section 6.8 paragraph 1). Thus, the general corrosion rate enhancement factor will be sampled from a uniform distribution with an upper bound of 2 and a lower bound of 1. The same upstream analysis recommends that, while bacteria preferentially colonize weldments, heat affected zones, and charged regions, it should be assumed that the general corrosion rate enhancement factor is uniformly distributed with respect to areal distribution (i.e., MIC enhanced corrosion could occur anywhere on the waste package surface) (CRWMS M&O 2000e, Section 6.8 paragraph 5). This technical product input information requires confirmation as discussed in Section 7.

4.1.11 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model

The Waste Package Outer Barrier Aging and Phase Instability Model requires a general corrosion rate multiplier to model the effect of aging and phase instability. These data and their sources are listed in Table 11.

According to the upstream analysis entitled *General and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.7.3 paragraph 2), general corrosion rates will be enhanced to model the effect of aging and phase stability. The upstream analysis goes on to recommend the general corrosion rate of the waste package outer barrier be enhanced by a factor between 1 and 2.5 (i.e., no enhancement up to the general corrosion rate being multiplied by 2.5) (CRWMS M&O 2000e, Section 6.7.3 paragraph 2). Thus, the general corrosion rate enhancement factor will be sampled from a uniform distribution with an upper bound of 2.5 and a lower bound of 1. This technical product input information requires confirmation as discussed in Section 7.

Table 11. Waste Package Outer Barrier Aging and Phase Instability Model Parameters and Their Sources

Parameter Name	Parameter Value	Source
General Corrosion Multiplier Distribution	Uniform over the range (1, 2.5)	CRWMS M&O 2000e Section 6.7.3

4.1.12 Waste Package and Drip Shield Exposure Conditions

The waste package and drip shield exposure conditions (relative humidity (RH), temperature, dripping water exposure period(s) and dripping water chemistry) are input to the WAPDEG DLL (see Section 6.3.16). The preparation and documentation of these data are included in the upstream analyses that serve as inputs to this analysis (CRWMS M&O 2000k, 2000l, and 2000m) (DTN: SN0001T0872799.006, MO0002SPALOO46.010, MO9911SPACDP37.001). This technical product input information requires confirmation as discussed in Section 7. See Attachment IV for further discussion of these inputs and their preparation.

4.2 CRITERIA

This section provides a summary of the NRC review and acceptance criteria outlined in the Issue Resolution Status Report (IRSR) that applies to the Container Life and Source Term Key Technical Issues (KTIs) (NRC 1999). The following six subissues are identified in the IRSR (NRC 1999, Section 2.2).

(1) Consider the effects of corrosion processes on the lifetime of the containers (NRC 1999, Section 2.2).

(2) Consider the effects of phase instability of materials and initial defects on the mechanical failure and lifetime of the containers (NRC 1999, Section 2.2).

(3) Evaluate the rate at which radionuclides in spent nuclear fuel (SNF) are released from the Engineered Barrier System (EBS) through the oxidation and dissolution of spent fuel (NRC 1999, Section 2.2).

(4) Evaluate the rate at which radionuclides in high-level waste (HLW) glass are leached and released from the EBS (NRC 1999, Section 2.2).

(5) Consider the effect of in-package criticality on waste package (WP) and EBS performance (NRC 1999, Section 2.2).

(6) Analyze the effects of alternate EBS design features on container lifetime and radionuclide release from the EBS (NRC 1999, Section 2.2).

Of these subissues, only subissues (1) and (2) are relevant to this analysis.

4.2.1 Acceptance Criteria Applicable To All Six Subissues

(1) The collection and documentation of data, as well as development and documentation of analyses, methods, models, and codes, are accomplished under approved quality assurance and control procedures and standards (NRC 1999, Section 4.0).

(2) Expert elicitation's, when used, are conducted and documented in accordance with the guidance provided in NUREG-1563 (Kotra, et. al., 1996) or other acceptable approaches (NRC 1999, Section 4.0).

(3) Sufficient data (field, laboratory, and natural analog) are obtained to adequately define relevant parameters for the models used to evaluate performance aspects of the subissues (NRC 1999, Section 4.0).

(4) Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) are used to determine whether additional data would be needed to better define ranges of input parameters (NRC 1999, Section 4.0).

(5) Parameter values, assumed ranges, test data, probability distributions, and bounding assumptions used in the models are technically defensible and can reasonably account for known uncertainties (NRC 1999, Section 4.0).

(6) Mathematical model limitations and uncertainties in modeling are defined and documented (NRC 1999, Section 4.0).

(7) Primary and alternative modeling approaches consistent with available data and current scientific understanding are investigated and their results and limitations considered in evaluating the subissue (NRC 1999, Section 4.0).

(8) Model outputs are validated through comparisons with outputs of detailed process models, empirical observations, or both (NRC 1999, Section 4.0).

(9) The structure and organization of process and abstracted models adequately incorporate important design features, physical phenomena, and coupled processes (NRC 1999, Section 4.0).

4.2.2 Acceptance Criteria For Subissue 1

(1) Identify and consider likely modes of corrosion for container materials, including dry-air oxidation, humid-air corrosion, and aqueous corrosion processes, such as general corrosion, localized corrosion, microbial-induced corrosion (MIC), stress corrosion cracking (SCC), and hydrogen embrittlement, as well as the effect of galvanic coupling (NRC 1999, Section 4.1.1).

(2) Identify the broad range of environmental conditions within the WP emplacement drifts that may promote the corrosion processes listed previously, taking into account the possibility of irregular wet and dry cycles that may enhance the rate of container degradation (NRC 1999, Section 4.1.1).

(3) Demonstrate that the numerical corrosion models used are adequate representations, taking into consideration associated uncertainties, of the expected long-term behaviors and are not likely to underestimate the actual degradation of the containers as a result of corrosion in the repository environment (NRC 1999, Section 4.1.1).

(4) Consider the compatibility of container materials, the range of material conditions, and the variability in container fabrication processes, including welding, in assessing the performance expected in the container's intended waste isolation function (NRC 1999, Section 4.1.1).

(5) Justify the use of data collected in corrosion tests not specifically designed or performed for the Yucca Mountain repository program for the environmental conditions expected to prevail at the Yucca Mountain site (NRC 1999, Section 4.1.1).

(6) Conduct a consistent, sufficient, and suitable corrosion-testing program at the time of the LA submittal. In addition, DOE shall identify specific plans for further testing to reduce any significant area(s) of uncertainty as part of the performance confirmation program (NRC 1999, Section 4.1.1).

(7) Establish a defensible program of corrosion monitoring and testing of the engineered subsystems components during the performance confirmation period to assure they are functioning as intended and anticipated (NRC 1999, Section 4.1.1).

4.2.3 Acceptance Criteria for Subissue 2

(1) Identify and consider the relevant mechanical failure processes that may affect the performance of the proposed container materials (NRC 1999, Section 4.2.1).

(2) Identify and consider the effect of material stability on mechanical failure processes for the various container materials as a result of prolonged exposure to the expected range of temperatures and stresses, including the effects of chemical composition, microstructure, thermal treatments, and fabrication processes (NRC 1999, Section 4.2.1).

(3) Demonstrate that the numerical models used for container materials stability and mechanical failures are effective representations, taking into consideration associated uncertainties, of the expected materials behavior and are not likely to underestimate the actual rate of failure in the repository environment (NRC 1999, Section 4.2.1).

(4) Consider the compatibility of container materials and the variability in container manufacturing processes, including welding, in its WP failure analyses and in the evaluation of radionuclide release (NRC 1999, Section 4.2.1).

(5) Identify the most appropriate methods for nondestructive examination of fabricated containers to detect and evaluate fabrication defects in general and, particularly, in seam and closure welds (NRC 1999, Section 4.2.1).

(6) Justify the use of material test results not specifically designed or performed for the Yucca Mountain repository program for environmental conditions (i.e., temperature, stress, and time) expected to prevail at the proposed Yucca Mountain repository (NRC 1999, Section 4.2.1).

(7) Conduct a consistent, sufficient, and suitable materials testing program at the time of the License Application submittal. In addition, DOE has identified specific plans for further testing to reduce any significant area(s) of uncertainty as part of the performance confirmation program (NRC 1999, Section 4.2.1).

(8) Establish a defensible program of monitoring and mechanical testing of the engineered subsystems components, during the performance confirmation period, to assure they are functioning as intended and anticipated, in the presence of thermal and stress perturbations (NRC 1999, Section 4.2.1).

4.3 CODES AND STANDARDS

The acceptance criteria listed above are consistent with the methodology described in the ASTM Standard Practice C-1174 for prediction of the long-term behavior of EBS components in a geologic repository (ASTM C 1174-97 1997).

5. ASSUMPTIONS

None of the following assumptions require confirmation prior to the use of the parameters developed in this document.

5.1 WASTE PACKAGE AND DRIP SHIELD DESIGN INPUT

The following assumptions are made for titanium grade 7 drip shield corrosion degradation modeling relevant to design inputs:

- The drip shield (DS) is assumed as an approximation to be composed of three parts; two vertical parallelepipeds (the drip shield side plates) and one horizontal parallelepiped (the drip shield top) each 15 mm thick. The surface area of the drip shield is therefore

$$DS\ Surface\ Area = 2 \cdot (2521 \cdot 4775) + (2512 \cdot 4775) = 3.607 \cdot 10^{7}\ \ mm^{2} \qquad \text{(Eq. 12)}$$

  This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6. This assumption has no effect on the results of this analysis. The WAPDEG code outputs the number of pit, crack, and patch penetrations versus time. The patch and drip shield surface areas are used only to determine the number of patches per drip shield to be simulated.

- The variability in drip shield degradation is adequately characterized by modeling 400 waste package/drip shield pairs with 500 patches per drip shield. This assumption results in a drip shield patch area of 7.214E+04 mm^2. While this assumption is based on analyses documented in Section 6.3.3. This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6. While this assumption is generally non-conservative relative to the use of a larger number of patches per drip shield (more stochastic samples considered), it is shown in Figure 6 of Section 6.3.3, that results obtained using 500 patches per drip shield are virtually indistinguishable from those for a larger number of patches.

The following assumptions are made for Alloy 22 waste package outer barrier corrosion degradation modeling relevant to design inputs:

- The waste package is assumed to be the "Single CRM 21-PWR Waste Package" identified by Waste Package Operations in a recent Design Input Transmittal PA-WP-99294.T (CRWMS M&O 1999c). The waste package surface area is based on the outer shell dimensions. The surface area of the waste package is therefore

$$WP\ Surface\ Area = 2 \cdot \pi \cdot \left({}^{1564}\!/\!_{2} \cdot 4775 \right) = 2.346 \cdot 10^{7}\ \ mm^{2} \qquad \text{(Eq. 13)}$$

  This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6. This assumption has no effect on the results of this analysis. The WAPDEG code outputs the number of pit, crack, and patch penetrations versus time. The patch and waste package surface areas are used only to determine the number of patches per waste package to be simulated.

- The variability in waste package outer barrier degradation is adequately characterized by modeling 400 waste package/drip shield pairs with 938 patches per waste package. This assumption results in a waste package patch area of 2.500E+04 mm^2. Based on the discussion of the similar drip shield modeling assumption above, in which it was found that WAPDEG results obtained using 500 patches per drip shield are virtually indistinguishable from those for a larger number of drip shield patches, it is concluded that the use of 938 patches for the waste package, almost twice that used for the drip shield, is a reasonable number to use. This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 5. While this assumption is generally non-conservative relative to the use of a larger number of patches per waste package (more stochastic samples considered), it is reasonable based on the argument presented for the drip shield.

- The weld filler metal used for the Alloy 22 waste package outer barrier lid welds is assumed to be Alloy 22. This assumption is consistent with CRWMS M&O 2000n, Section 6.3 in which it is stated that "Filler metal material shall be selected to be compatible with the base material." This assumption is used in the WAPDEG degradation models through the use of model parameters appropriate for Alloy 22 in the weld regions.

The following assumptions are made for the 316NG stainless steel waste package inner barrier degradation modeling:

- The stainless-steel waste-package inner layer, which is to provide structural support to the waste package, was not included in the analysis. Although it would provide a certain level of performance for waste containment and potentially act as a barrier to radionuclide transport after waste package breach, the potential performance credit of the stainless-steel layer was not included in the nominal TSPA-SR analysis. This assumption is conservative.

These assumptions are used in the formulation of the WAPDEG Model.

5.2 RELATIVE HUMIDITY THRESHOLD

- The relationship between the critical threshold RH and exposure temperature is based on the assumption of the presence of a sodium nitrate ($NaNO_3$) salt film on the waste package and drip shield surface (see Section 4.1.2). The sodium nitrate salt film is assumed to be present in the absence or presence of dripping water. This assumption is conservative. This assumption is used throughout the analysis.

5.3 LOCALIZED CORROSION OF DRIP SHIELD

- It is assumed that localized corrosion (LC) is not possible on the titanium grade 7 drip shield under all expected repository conditions. This assumption is based on results and conclusions of upstream analyses (CRWMS M&O 2000d, Section 7.1) which were reproduced in Figure 2. Localized corrosion is considered to initiate when *Ecorr* exceeds *Ecrit* (i.e., • *E* < 0). From Figure 2, this can not happen even if exposure *pH* exceeds 14 based on the -4• confidence interval shown. This assumption is consistent with the available data. This assumption is used throught the analysis.

- It is assumed that the unqualified data for the localized corrosion rate of Titanium grade 7, given by the distribution presented in Section 4.1.6 and Table 3, can be used in this analysis.

This data is a conservative representation of localized corrosion rate of Titanium grade 7 under repository conditions. The basis of this assumption is that the lower bound of the localized corrosion rate distribution presented in Table 3 is based on a localized corrosion rate measured in a 19% HCl + 4% $FeCl_3$ + 4% $MgCl_2$ solution at 82°C and the upper bound is based on a localized corrosion rate measured in boiling 3:1 Aqua Regia solution (CRWMS M&O 2000f, Table 16). These values are “more severe” (CRWMS M&O 2000f, Section 6.7 paragraph 4) than Titanium grade 7 localized corrosion rates measured in deaerated brine at 90°C. Hence the use of this data to model Titanium grade 7 localized corrosion in the proposed resository is conservative. Furthermore, as stated in the previous assumption, localized corrosion of the drip shield will never initiate under expected repository exposure conditions. Therefore, this assumption has no impact on the results of this analysis. This assumption is used in Section 4.1.6.

5.4 LOCALIZED CORROSION OF WASTE PACKAGE OUTER BARRIER

- While it could be assumed that localized corrosion (LC) is not possible on the Alloy 22 waste package outer barrier for the same reasons as the titanium grade 7 drip shield, that assumption was not made. Instead, localized corrosion models and initiation criteria from upstream analysis (CRWMS M&O 2000d) were implemented into the WAPDEG_Inputs element (see Figure 6), even though, based on conclusions of the upstream analyses (CRWMS M&O 2000d, CRWMS M&O 2000e), localized corrosion of the Alloy 22 waste package outer barrier can never occur under repository relevant exposure conditions (see Figure 1). Inclusion of localized corrosion models and initiation criteria for the Alloy 22 outer barrier allows for easier implementation of sensitivity studies should the need arise. This assumption has no impact on the results of this analysis.

- In the current analysis, localized corrosion of the waste package outer barrier is assumed to initiate only under dripping conditions. This is because of the necessary presence of aggressive ions (such as chloride) in order to initiate and sustain pit and crevice growth, and because the only mechanism for these ions to gain ingress to the drift is through drips. This assumption has no impact on the results of this analysis given the previous paragraph. This assumption is used throughout this analysis.

- It is assumed that dripping water resulting from condensation on the underside of the drip shields (if it occurs) does not lead to initiation of localized corrosion. The basis of this assumption is that the condensed water does not have the aggressive aqueous chemistry associated with dripping water from other sources. This assumption is used in the WAPDEG Model in that localized corrosion of the Alloy 22 waste package outer barrier is not allowed to initiate in the absence of dripping water contact through a failed drip shield (i.e., the waste package is assumed to undergo humid-air corrosion only while the dripshield remains unbreached).

- The localized corrosion rates for Alloy 22 (Table 2) are assumed to be loguniformly distributed. The basis for this assumtion is that the values in Table 2 span three orders of magnitude and the percentiles provided are consistent with a loguniform distribution. This assumption is used in the localized corrosion for the Alloy 22 waste package outer barrier and lids. This assumption has no impact on the results of this analysis.

- It is assumed that the unqualified data for the localized corrosion rate of Alloy 22, given by the distribution presented in Section 4.1.5 and Table 2, can be used in this analysis. This data is a conservative representation of localized corrosion rate of Alloy 22 under repository conditions. The basis of this assumption is that the upstream analysis (CRWMS M&O 2000e, Section 6.6.6) from which the data was obtained indicates that "This distribution reasonably bounds those extreme penetration rates found in the literature . . ." Hence the use of this data to model Alloy 22 localized corrosion in the proposed resository is conservative. This assumption is used in Section 4.1.5.

5.5 MANUFACTURING DEFECTS IN CLOSURE-LID WELDS

The major assumptions used to develop the abstraction for the probability of the occurrence and size of manufacturing defects in the waste package closure-lid welds are given below. Details of the assumptions employed are described in the companion calculation (CRWMS M&O 2000g).

- Only surface breaking defects are considered. There is uncertainty associated with this assumption because, as general corrosion propagates, some of the existing surface-breaking defect flaws may disappear and some of the embedded defects may become surface-breaking defects. This evolution of the surface-breaking defects was not considered. This assumption could be nonconservative if the number of exposed previously embedded defect flaws exceeds the number of initially suface-breaking flaws at a given time during the simulation. The results of this analysis, particularly Section 6.4, indicate that first crack penetration times are earlier than first patch penetration times only for failure profiles above the 75^{th} percentile, i.e., crack penetration is not the dominant failure mode in the current analysis. Therefore, this assumption does not have significant impact on the analysis results. This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- Only the closure-lid weld of the waste package develops residual stresses high enough to cause stress corrosion cracking. Other fabrication welds used in waste package fabrication are fully annealed prior to waste emplacement, and thus do not develop residual stress high enough for stress corrosion cracking to occur (CRWMS M&O 2000h, Section 5, Assumption 1). This assumption is consistent with available data. This assumption is used in the WAPDEG Model by restricting Stress Corrosion Cracking processes to occur only on that fraction of waste package patches that are considered closure weld patches (Sections 6.3 and 6.4).

- Defects are assumed to be spatially randomly distributed as represented by a Poisson process (CRWMS M&O 2000g). This assumption is consistent with available data. This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- The mean flaw density (Poisson distribution parameter) of the closure-lid weld, 0.6839 flaws/meter, is assumed to be as given in CRWMS M&O (2000o, Section 6.2.1) (DTN: MO9910SPAFWPWF.001). This is a reasonable value based on the literature reviewed in CRWMS M&O 2000o. This assumption is neither conservative nor nonconservative. This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- The fraction of surface breaking flaws is assumed to be uniformly distributed between the minimum and maximum fractions used to determine the average fraction quoted in CRWMS M&O 2000o (DTN: MO9910SPAFWPWF.001). The basis of this assumption is that the three values quoted (0.13%, 0.40% and 0.49%) in the analyses are not sufficient to determine a single representative average value (CRWMS M&O 2000g). The use of the uniform distribution is a reasonable representation of the uncertainty in expressing this value. This assumption is consistent with available data and analyses (CRWMS M&O 2000o, CRWMS M&O 2000g). This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- Pre-inspection flaw sizes are assumed to be lognormally distributed, with distribution parameters (dependent on the weld thickness) as given in CRWMS M&O (2000o, Section 6.2.1) (DTN: MO9910SPAFWPWF.001). This assumption is consistent with available data and analyses. This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- The probability of non-detection (PND) is given as a function of flaw size as discussed in CRWMS M&O 2000o (DTN: MO9910SPAFWPWF.001). The model is dependent on the following parameters: the detection threshold (*p*), the location parameter (*b*), and the scale parameter (•). The *b* and • parameters are taken to be uncertain with a uniform distribution (see Section 4.1.7). The ranges for these distributions are determined from the values identified in the literature quoted in CRWMS M&O 2000o (DTN: MO9910SPAFWPWF.001). This is a reasonable assumption, as these values are based on similar industrial manufacturing practices as reviewed in the upstream analysis (CRWMS M&O 2000o). This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

- It is assumed that all flaws detected are repaired to specified acceptance criteria or removed in such a manner that they are eliminated from consideration for further failure analysis. This assumption is consistent with upstream analysis (CRWMS M&O 2000o, Section 5.1). This assumption is used in the analysis of manufacturing defects in waste package closure-lid welds in the WAPDEG Model (Sections 6.3 and 6.4).

5.6 STRESS AND STRESS INTENSITY FACTOR PROFILES IN CLOSURE-LID WELDS

The following assumptions were used to develop abstractions for stress and stress intensity factor profiles in the closure-lid welds (outer and inner lids) of the outer barrier of the waste package. Details of the assumptions employed and the abstraction analyses are given in the companion AMR (CRWMS M&O 2000i).

- It is assumed that all fabrication welds of the waste package, except the welds for the closure lids, are not subject to SCC. The basis of this assumption is that all welds, except the welds for the closure lids, are fully annealed before the waste packages are loaded with waste

(CRWMS M&O 2000n, Section 8.1.7). This assumption is consistent with one used in the upstream analysis (CRWMS M&O 2000h, Section 5). This assumption is used in the WAPDEG Model in that SCC processes are only allowed to occur on those patches with closure lid welds on them.

- The hoop stress (and the corresponding stress intensity factor for radial cracks) is the prevailing stress in the closure-lid welds that fail the waste packages by SCC, if it occurs. Thus, the abstraction is limited to the profiles for the hoop stress and corresponding stress intensity factor for radial cracks. This assumption is conservative. The hoop stress profiles supplied are more severe than the radial or longitudinal stress profiles (CRWMS M&O 2000h, Attachment I). This assumption is used in the WAPDEG Model in the stress profiles used in the Slip Disolution Abstraction Model.

- The hoop stress and corresponding stress intensity factor profiles in the outer barrier inner lid welds from the process-level analysis are for a plane that is inclined at an angle of 37.5° with the outer surface of the outer barrier inner lid (CRWMS M&O 2000h). Because the SCC analysis in the integrated waste package degradation model (WAPDEG) assumes that cracks propagate in the direction of the normal to the lid surface, the profiles from the process-level analysis were projected to the plane normal to the outer surface of the lid. It is assumed the SCC analysis with the "simple" projection of the profiles represents the hoop stress and stress intensity factor profiles for the inclined plane. This assumption is consistent with the upstream analysis. This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model inputs (see Section 6.3.12.1).

- The hoop stress and corresponding stress intensity factor profiles as a function of depth in the closure-lid welds from the process-level analyses represent the mean profiles. The uncertainties in the hoop stress and corresponding stress intensity factor profiles are represented with normal distribution, and the uncertainty range is bounded within three standard deviations (± 3 s.d's) around the mean profiles. This assumption is consistent with upstream analysis (CRWMS M&O 2000h, Section 6.2.2.5). This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model inputs (see Section 6.3.12.1).

- The hoop stress and stress intensity factor profiles vary along the circumference of the closure-lid welds, and those represent the variability in the profiles for a given waste package. It is assumed that the same degree of the profile variability is applied equally to all the waste packages in the repository, and there is no variability in the profiles among waste packages. This assumption is consistent with upstream analysis (CRWMS M&O 2000h, Section 6.2.2.5). This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model inputs (see Section 6.3.12.1).

- As a crack propagates in the closure lid welds or the welds are corroded, stresses in the welds may re-distribute such a way that the SCC initiation and crack growth are mitigated (CRWMS M&O 2000h). Such a stress re-distribution or relaxation is not considered in the current abstraction. This is a conservative approach. This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model (see Section 6.3.12.1).

5.7 SLIP DISSOLUTION MODEL

The following assumptions were used to develop the abstractions for the slip dissolution model for the SCC crack initiation and growth. Details of the assumptions employed and the abstraction analyses are described in the companion abstraction AMR (CRWMS M&O 2000i).

- Induction-heating solution annealing is used to mitigate residual stress in the outer closure-lid welds, and laser peening is used in the outer barrier inner closure-lid welds of the outer barrier. The manufacturing defect analyses (CRWMS M&O 2000o) and the abstraction calculation (CRWMS M&O 2000g) are assumed applicable to the closure-lid welds after the stress mitigation processes. This assumption is consistent with upstream analysis (CRWMS M&O 2000i). This assumption is conservative in that the effect of annealing is generally to blunt defect asperities and lessen the severity of stress states around defects. This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model.

- It is assumed that the analyses for incipient cracks reported in (CRWMS M&O 2000h) are applicable to the closure-lid welds after the stress mitigation process. This assumption is consistent with upstream analysis. This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model.

- An exponential distribution with a maximum size of 50 µm and a median size of 20 µm was suggested for the incipient crack size distribution (CRWMS M&O 2000h, Section 6.5.2). In this analysis, the maximum crack size (50 µm or 0.05 mm) is used for all the incipient cracks considered in the SCC analysis. This is a conservative assumption. This assumption is used in the WAPDEG Model in the Slip Dissolution Abstraction Model (see Sections 4.1.9 and 6.3.13).

- It is assumed that the drip shield is not subject to stress corrosion cracking (SCC). This assumption is based on conclusions of upstream analyses (CRWMS M&O 2000h, Section 5). This assumption is used in the WAPDEG Model in that no SCC model input is supplied to the WAPDEG Model and thus, no SCC of the drip shield is allowed to occur.

- It is assumed that SCC of the of the waste package outer barrier closure lid welds can initiate as soon as the relative humidity threshold is satisfied. The basis of this assumption is that SCC requires the presence of a stable water film. This assumption is used in the Slip Dissolution Abstraction Model.

5.8 EFFECT OF MICROBIOLOGICALLY INFLUENCED CORROSION (MIC)

The following assumptions were used for the effect of microbiologically influenced corrosion (MIC) of the drip shield (Titanium grade 7) and waste package outer barrier (Alloy 22).

- The drip shield is assumed not subject to microbiologically influenced corrosion (MIC). The basis of this assumption is given in CRWMS M&O (2000f, Sections 5.8 and 6.9) in which it is stated that the effect of microbial growth on the corrosion potential is not significant and the initiation of crevice corrosion under bio-films formed on titanium has never been observed. This assumption is used in the WAPDEG Model in that no MIC model input is supplied to the WAPDEG Model and thus, no MIC of the drip shield is allowed to occur.

- The waste package outer barrier is assumed subject to MIC when RH is greater than 90%. The basis of this assumption is given in CRWMS M&O (2000e, Section 6.10) in which it is stated that corrosion rates will be enhanced to account for MIC above 90% RH. This assumption is used in the WAPDEG Model in the MIC Abstraction Model input parameters (see Section 6.3.14.1).

- It is assumed that the effect of MIC on corrosion degradation of the waste package outer barrier is represented by a general corrosion enhancement factor. The enhancement factor is assumed to have uniform distribution between one and two. The basis of this assumption is described in CRWMS M&O (2000e, Section 6.8) in which it is stated that the general corrosion rate enhancement factor is uniformly distributed between one and two. This assumption is used in the WAPDEG Model in the MIC Abstraction Model input parameters (see Section 6.3.14.1).

- It is assumed that the MIC general corrosion enhancement factor for the waste package outer barrier varies among waste packages and among patches for a given waste package. The basis of this assumption is given in CRWMS M&O (2000e, Section 6.8).

5.9 EFFECT OF AGING AND PHASE INSTABILITY

The following assumptions were used for the effect of aging and phase instability on corrosion degradation of the drip shield (Titanium grade 7) and waste package outer barrier (Alloy 22).

- The drip shield is assumed immune to long-term aging and phase instability under the thermal conditions expected in the repository. The basis of this assumption is given in CRWMS M&O (2000f, Section 5.9) in which it is stated that the effects of phase instability on degradation of Titanium grade 7 are expected to be insignificant. While Titanium grade 7 does contain small additions of Palladium (Pd), Titanium-Palladium intermettallic compounds have not been reported to form in Titanium grade 7 under normal heat treatments. This assumption is used in the WAPDEG Model in that no Aging and Phase Instability Abstraction Model input is supplied for the Titanium grade 7 drip shield, thus there is no effect of aging and phase instability on the drip shield degradation characteristics.

- It is possible that the waste package outer barrier can be subject to long-term thermal aging and phase instability under the repository thermal conditions. It is assumed that the thermal aging effect on corrosion degradation of the waste package outer barrier is represented by a general corrosion enhancement factor. The enhancement factor is assumed to have uniform distribution between the limits of 1 and 2.5. The basis of this assumption is described in CRWMS M&O (2000e, Sections 5.9 and 6.7) in which it is stated that the general corrosion rate enhancement factor due to the effects of aging and phase stability is assumed to have uniform distribution between the limits of 1 and 2.5. This assumption is used in the Aging and Phase Instability Abstraction Model input (see Section 6.3.15.1).

- It is assumed that the general corrosion enhancement factor for the thermal aging of the waste package outer barrier varies among waste packages and among patches for a given waste package. The basis of this assumption is given in CRWMS M&O (2000e, Section 6.7) in which it is stated that the distribution (uniform distribution between the limits of 1 and 2.5) is one-half uncertainty and one-half variability. This is implemented in the WAPDEG Model in the Aging and Phase Instability Abstraction Model input (see Section 6.3.15.1) by assigning an uncertain share of variance of this distribution to waste-package-to-waste-package variance and patch-to-patch variance through the use of the variance partitioning procedures within the WAPDEG code (see Section 6.3.17).

5.10 EFFECT OF RADIOLYSIS

- Both the drip shield (Titanium grade 7) and waste package outer barrier (Alloy 22) are assumed not to be subject to radiolysis-enhanced corrosion under the expected repository conditions. The basis of this assumption is described in the companion AMRs: Sections 5.7 and 6.8 of CRWMS M&O 2000f for the drip shield and Sections 5.7 and 6.4.4 of CRWMS M&O 2000e for the waste package outer barrier. To summarize, the shift in corrosion potential due to gamma radiolysis will be less than 200 mV and this shift in corrosion potential is insufficient to cause localized corrosion initiation (also see Figure 1 and Figure 2). This assumption is consistent with the upstream analysis. This assumption is used in the WAPDEG Model in that no effect of radiolysis is included in the model.

5.11 HYDROGEN INDUCED CRACKING (HIC) OF DRIP SHIELD

- It is assumed that the titanium grade 7 drip shield is not subject to hydrogen induced cracking (HIC) under repository exposure conditions. The basis of this assumption is described in CRWMS M&O 2000j in which it is concluded that the hydrogen concentration in the Titanium grade 7 drip shield will never surpass 400 • g/g (a conservative threshold value for the onset of HIC). This assumption is consistent with the upstream analysis. This assumption is used in the WAPDEG Model in that no HIC Model input is provided for the drip shield.

6. ANALYSIS/MODEL

This section provides descriptions for the approach to and the conceptual model for the waste package and drip shield degradation analysis using the WAPDEG Model. The implementation of the abstraction models of the process-level models for the corrosion degradation processes considered is described. Then the WAPDEG analysis results are discussed in terms of a set of profiles for the waste package and drip shield failure and penetration openings as a function of time.

6.1 APPROACH TO WASTE PACKAGE AND DRIP SHIELD DEGRADATION ANALYSIS

The TSPA-SR subsystem model for evaluating degradation of the waste package and drip shield is the WAste Package DEGradation (WAPDEG) model (CRWMS M&O 1999e). The WAPDEG Model is based on a stochastic simulation approach and provides a description of waste package and drip shield degradation, which occurs as a function of time and repository location for specific design and thermo-chemical-hydrologic exposure conditions. [For a convenience of discussion in this section, the drip shield is considered to be an integral part of the waste package, and no separate discussion is given for the drip shield.] The purposes of the stochastic approach and WAPDEG Model are three fold:

Provide realistic representation of waste package degradation processes in the repository (rather than taking an excessively conservative approach that is routinely chosen to simplify the analysis);

Capture the effects of variation and uncertainty both in exposure conditions and degradation processes over a geologic time scale; and

Perform analysis within reasonable computational resources and time.

Abstractions of the process-level models for implementation in the WAPDEG Model were developed in such a way that important features of the process-level models are captured as explicitly as possible, and that the degradation processes and their characteristics are properly represented in the waste package degradation analysis.

The TSPA-SR waste package degradation analysis simulates the behavior of a few hundred waste packages (see Sections 5.1 and 6.3). Effects of spatial and temporal variations in the exposure conditions over the repository were modeled by explicitly incorporating relevant exposure condition histories into the waste package degradation analysis. The exposure condition parameters that were considered varying over the repository are relative humidity and temperature at the waste package surface, seepage into the emplacement drift, and the chemistry of the seepage water. In addition, potentially variable corrosion processes within a single waste package were represented by dividing the waste package surface into "patches" and populating stochastically the corrosion model parameter values and/or corrosion rates over the patches. The model parameter values and corrosion rates were sampled from their variance, which is dictated by the range of the expected local exposure conditions. The "patches" approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package at a given time.

The TSPA-SR analysis has incorporated more explicit representation (than previous TSPA analyses) of the uncertainty and variability in waste package degradation (waste package failure and penetration number profiles). For the corrosion models and parameters for which data and analyses are available, their uncertainty and variability were quantified and implemented into the WAPDEG analysis. For other models and parameters for which the uncertainty and variability is not quantifiable, the variance in their value was assumed (see Section 6.3.17), or the entire variance was used as uncertainty. The sources and/or processes that may contribute to *uncertain* variability in corrosion processes may include local (or micro-scale) chemistry of solution contacting waste package, temporally and spatially varying long-term post-closure exposure conditions (such as water dripping), manufacturing of waste package, variation of the materials properties (especially microstructure-scale), etc.

In the TSPA-SR analysis, waste package degradation was analyzed with multiple realizations of WAPDEG for the uncertainty analysis of the uncertain corrosion parameters—each WAPDEG realization corresponding to a complete WAPDEG run for a given number of waste packages. Accordingly, each of the WAPDEG analysis outputs discussed above (i.e., waste package failure time, crack penetration number, pit penetration number, and patch penetration number) are reported as a group of "degradation profile curves" that represent the potential range of the output parameters. For example, the waste-package failure time profiles are reported with a group of "curves" for the cumulative probability of waste package failures as a function of time—each curve corresponding to the failure time profile from one WAPDEG realization (or one complete WAPDEG run).

6.2 CONCEPTUAL MODEL FOR WAPDEG ANALYSIS OF WASTE PACKAGE AND DRIP SHIELD

In the TSPA-SR analysis, WAPDEG Models various types of corrosion mechanisms that may occur on a waste package and drip shield as a function of the exposure time and conditions. [For convenience of discussion in this Section, the drip shield is considered to be an integral part of the waste package. Except where it is necessary, no separate discussion is given for the drip shield.] In the nominal case analysis of TSPA-SR, the waste package outer barrier (WPOB) and drip shield were included in the waste package degradation analysis. The stainless-steel waste-package inner layer, which is to provide structural support to the waste package, was not included in the analysis. Although it would provide a certain level of performance for waste containment and potentially act as a barrier to radionuclide transport after waste package breach, the potential performance credit of the stainless-steel layer was ignored in the nominal TSPA-SR analysis.

In this analysis, a humid-air corrosion condition is defined as an exposure condition for which the RH at the waste package surface is equal to or greater than the threshold RH in the absence of drips. An aqueous corrosion condition requires the presence of dripping water. Corrosion and other degradation processes and their models and parameters that have been incorporated into the TSPA-SR waste package degradation analysis are described below.

- Threshold relative humidity (RH) for corrosion initiation. The threshold RH is based on the deliquescence point of $NaNO_3$ salt and is a function of exposure temperature (see Sections 3.2.3 and 4.1.2). The same threshold RH is used for both the dripping and non-dripping cases (see Section 5.2). It is assumed that a stable water layer on the surface that can support electrochemical reactions of corrosion forms if the RH is equal to or greater than the threshold RH.

- Humid-air and aqueous general corrosion rate of waste package outer barrier. The same general corrosion rate is used for both aqueous and humid-air general corrosion.

- Humid-air and aqueous general corrosion rate of drip shield. The same general corrosion rate is used for both aqueous and humid-air general corrosion.

- Localized corrosion (pitting and crevice corrosion) initiation threshold for the waste package outer barrier, which is based on the corrosion potential (E_{corr}) and threshold corrosion potential (E_{th}) as a function of the contacting solution pH. If $E_{corr} \geq E_{th}$, localized corrosion initiates. Localized corrosion also requires the presence of dripping water (see Section 5.4). Localized corrosion ceases if the exposure condition changes such that E_{corr} becomes less than E_{th}.

- Localized corrosion (pitting and crevice corrosion) penetration rate for waste package outer barrier.

- Localized corrosion (pitting and crevice corrosion) of the drip shield is assumed not to occur (see Section 5.3).

- The hoop stress and corresponding radial-crack stress intensity factor versus depth in the outer barrier outer and inner closure-lid welds of the waste package.

- The Slip Dissolution Model for Stress Corrosion Cracking (SCC).

- Probability of occurrence and size of manufacturing defects in waste package outer barrier closure-lid welds and its effect on SCC.

- Threshold RH for the initiation of microbiologically influenced corrosion (MIC) of waste package outer barrier and the enhancement factor (uniform distribution between 1 and 2) for general corrosion rate due to MIC. The drip shield is assumed not to be subject to MIC.

- The enhancement factor (uniform distribution between 1 and 2.5) to the general corrosion rate for long-term aging and phase instability of waste package outer barrier. The drip shield is assumed not to be subject to thermal aging.

- Radiation enhanced corrosion of waste package outer barrier and drip shield. It was assumed that the waste package and drip shield are not subject to radiation enhanced corrosion under the repository conditions.

- Because both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift, both sides are subject to corrosion if the initiation threshold is met.

- When the waste package fails, the waste package degradation analysis also considers corrosion degradation of the waste package on its inner surface (inside-out corrosion). The inside-out corrosion analysis includes general corrosion and localized corrosion of the waste-package outer barrier. The inside-out corrosion would cause penetrations by general and localized corrosion in addition to those by outside-in corrosion only. The inside-out general corrosion is assumed to initiate at the time of the waste package failure. Like the outside-in localized corrosion, initiation of the inside-out localized corrosion is based on the corrosion potential and threshold corrosion potential, which are a function of the pH of water inside the breached waste package. The in-package water chemistry is determined from analysis of degradation of the waste form and other internal materials (such as basket materials) provided to the WAPDEG Model through the waste package and drip shield exposure conditions (see Section 4.1.12 and Attachment IV).

The drip shield was assumed not to be subject to SCC because it will be fully annealed before it is placed in the emplacement drift. Likewise, all the fabrication welds in the waste container, except the welds for the closure lids, were assumed fully annealed and thus not subject to SCC. Therefore, only the closure-lid welds were considered in the SCC analysis. It was assumed that SCC is operative on the closure-lid welds if the RH of the waste package surface is greater than the threshold RH. In addition, two alternative SCC models, the slip dissolution model and the threshold stress intensity factor model, were considered.

As discussed in detail in Section 6.2.2 of CRWMS M&O 2000h, a dual closure-lid design for the waste package outer barrier has been proposed to mitigate potential premature failure of waste packages by SCC. The dual closure-lids are referred to as the outer lid and inner lid, respectively, in this report. The outer lid is 25-mm thick and the inner lid is 10-mm thick. There is a physical separation between the two lids. Thus, any SCC cracks initiated in the outer closure-lid stop after penetrating it, and then the inner closure-lid welds are subject to the SCC crack initiation and growth. See Section 6.2.2 of CRWMS M&O 2000h for details of the design. A schematic of the dual closure-lid design is shown in Figure 4.

In order to implement the SCC processes in the dual closure-lids in an explicit way and capture the intended purpose of the dual lid design features in the waste package degradation analysis, the following modelling approach has been implemented within the WAPDEG Model.

- The waste package outer barrier is modeled as two layers, with their thicknesses being consistent with that of two closure lids: the “pseudo”-outer layer is 25-mm thick, and the “pseudo”-inner layer is 10-mm thick. The actual design thickness of the outer barrier is 20-mm (see Section 4.1.1). Figure 4 shows a schematic of the waste package configuration in the WAPDEG analysis to implement the SCC of the dual closure-lid welds.

- As illustrated in Figure 4, the general corrosion rate distribution that is applied to the “pseudo”-outer layer (25-mm thick) was constructed by increasing the original Alloy 22 general corrosion rate (see Section 4.1.4) by a factor of 2.5. Because the general corrosion rate is time-independent, this is equivalent to analyzing a 10-mm thick layer. Likewise, the localized corrosion penetration rate for the “pseudo”-outer layer was constructed by increasing the original penetration rate (Section 4.1.5) by a factor of 2.5. The Alloy 22 localized penetration rate is also time-independent. The original general and localized corrosion rate was applied to the outer layer closure-lid patches.

- The original general corrosion rate distribution (Section 4.1.4) and localized corrosion penetration rate (Section 4.1.5) were used for the “pseudo”-inner layer (10-mm thick) without modification. The same original general and localized corrosion rate was applied to the inner closure-lid patches.

- As discussed above, inside-out corrosion of the waste package, after an initial breach, is also included in the TSPA-SR waste package degradation analysis. The inside-out corrosion contributes to penetrations by general and localized corrosion in addition to those by the outside-in corrosion only. The number of penetration openings (or the number of penetration openings as a function of time) in the inner layer is used for the radionuclide release rate from the failed waste packages. For the purpose of the inside-out corrosion analysis, the "pseudo"-inner layer (10-mm thick) is treated as the actual outer barrier (20-mm thick). Thus, in the WAPDEG implementation, because the thickness of the "pseudo"-inner layer is defined as 10-mm, the general corrosion rate for the inside-out corrosion was constructed by decreasing the original Alloy 22 rate by a factor of 2. Likewise, the localized corrosion penetration rate for the inside-out corrosion was reduced by a factor of 2. This is equivalent to analyzing the inside-out corrosion of a 20-mm thick outer barrier. The same general and localized corrosion rate was used for inside-out corrosion of the inner closure-lid patches.

The exposure conditions that were included in the TSPA-SR waste-package degradation analyses are temperature and relative humidity at the waste package and drip shield surface, in-drift dripping water contact, and pH of the water contacting the waste package and drip shield. The temperature and relative humidity histories at the waste package and drip shield surface are provided from the thermal-hydrologic model abstraction (CRWMS M&O 2000k). The evolution of the water chemistry contacting the waste package and drip shield surfaces are provided in the *In-Drift Precipitates/Salts Analysis* (CRWMS M&O 2000l). The evolution of the exposure conditions inside the waste package is provided in the *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m).

In the analysis, the waste package surface RH is tested against the threshold RH (RH_{th}) for corrosion initiation of the drip shield (DS) and waste package outer barrier (WPOB). When the surface RH becomes greater than the threshold RH, the waste package and drip shield could undergo different corrosion degradation modes depending on whether they are dripped on or not.

For waste packages that are not dripped on, the waste package outer barrier (and drip shield) undergoes humid-air corrosion. Under humid-air conditions, the waste package outer barrier (and drip shield) undergoes general corrosion all the time and fails eventually by gradual thinning. As discussed in Sections 4.1.3 and 4.1.4, the general corrosion rates of the waste package outer barrier (and drip shield) are very low.

For waste packages and drip shields that are dripped on, the wetted areas (by drips) of the drip shield or waste package is assumed to undergo aqueous corrosion if the RH at the surface is greater than the threshold RH. If the RH at the waste package or drip shield surface is less than the threshold RH, the dripping water will evaporate resulting in exposure conditions more resembling those of humid-air than aqueous corrosion. It is also assumed that dripping water resulting from condensation on the underside of the drip shields (if it occurs) does not lead to the aggressive aqueous corrosion conditions associated with dripping water from other sources (i.e., the waste package is assumed to undergo humid-air corrosion only while the dripshield remains unbreached) (see Section 5.4). General corrosion occurs all the time under aqueous corrosion conditions. Initiation of localized (pitting and crevice) corrosion is dependent on the local exposure environment on the wetted patches. In the current analysis, localized corrosion of the waste package outer barrier is assumed to initiate only under dripping conditions (i.e., through a breached drip shield, see Section 5.4). Localized corrosion for a waste package outer barrier patch is assumed to initiate if the corrosion potential (E_{corr}) is greater than or equal to the threshold corrosion potential (E_{th}). After initiated, localized corrosion continues while $E_{corr} \geq E_{th}$. If E_{corr} becomes less than E_{th}, localized corrosion stops. As discussed previously (see Section 5.7), SCC of the waste package closure-lid welds was assumed operative as long as the RH is greater than the threshold RH, regardless of whether it is dripped on or not.

The WAPDEG analysis provides an assessment of corrosion degradation of waste packages for three types of penetration modes: crack penetration by SCC, (in the closure weld regions only) pit penetration by pitting and crevice corrosion, and large (or patch) opening by general corrosion. The analysis provides, as output, the cumulative probability of waste package failure by one of the three penetration modes as a function of time, and the number of penetrations for each of the penetration modes as a function of time. The waste package failure time and penetration number profiles are used as input to other analyses such as waste form degradation and radionuclide release rate from failed waste packages.

Schematic of Dual Closure Lids of Waste Package Outer Barrier

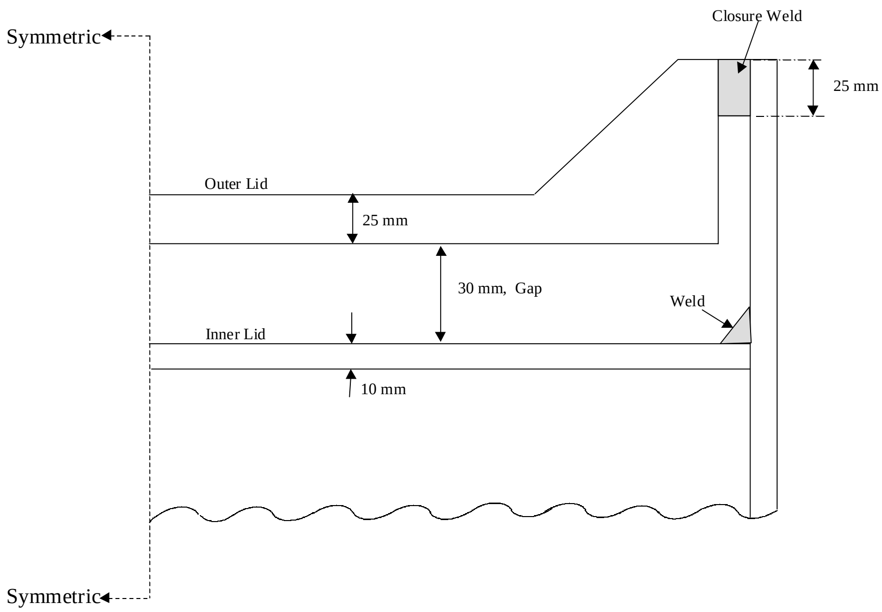

Figure 3. Schematic of Dual Closure-Lids of Waste Package Outer Barrier

WAPDEG Waste Package Configuration To Implement SCC of Closure-Lids

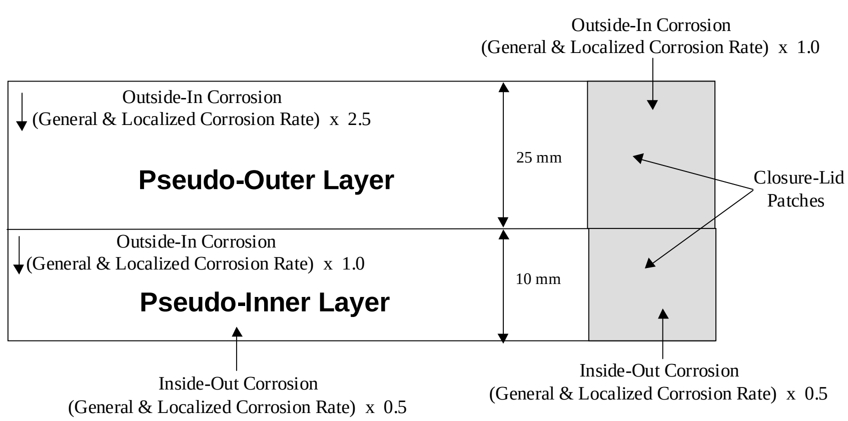

Figure 4. Schematic of Waste Package Configuration in WAPDEG Analysis to Implement SCC of Dual Closure-Lids of Waste Package Outer Barrier

6.3 IMPLEMENTATION OF CORROSION MODELS AND SIMULATION PARAMETERS

In the current analysis, the waste package degradation model is composed of two components; the WAPDEG dynamic-link library (WAPDEG DLL), which is responsible for modeling the variability in waste package degradation, and the implementation thereof in the GoldSim software (which calls the WAPDEG DLL and is responsible for treating the uncertainty in the parameters used by the WAPDEG DLL (CRWMS M&O 1999e)). Throughout this Section, reference will be made to various parts of the GoldSim (Golder Associates 2000) implementation as well as the various input files and parameters and parameter distributions used in waste package degradation modeling.

6.3.1 GoldSim Implementation Overview

A schematic of the GoldSim implementation, which calls the WAPDEG software, is shown in Figure 6.

WDSeed is a stochastic element characterized by a uniform distribution between 1 and 2^{31}-1 (the maximum positive 32-bit integer). WDSeed is used to generate a different integer for each GoldSim realization with which to seed the WAPDEG random number generator (note that the output of the WDSeed element is fed into the WAPDEG_Inputs element).

The number of waste packages per GoldSim realization (entered in the GoldSim data element labeled NumPak) was set at 400. Note that the output of the NumPak element is fed into the WAPDEG_Inputs element.

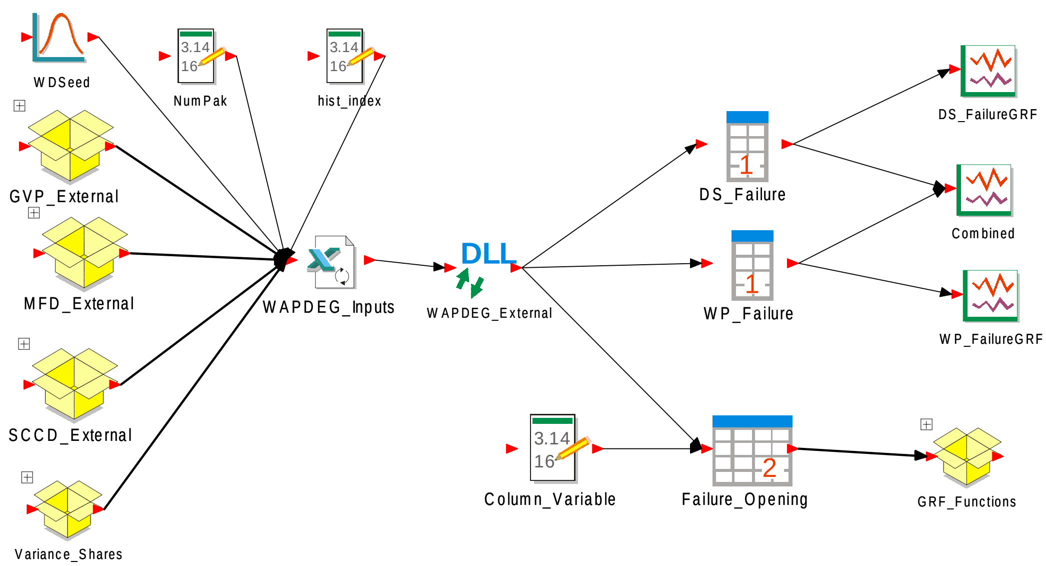

Figure 5. GoldSim implementation which calls the WAPDEG software.

The four GoldSim containers (not to be confused with waste containers) GVP_External, MFD_External, SCCC_External, and Variance_Shares shall be discussed later in this document in relation to their specific functions.

The Hst_Index data element contains the number 13. This represents the file index (line number in a file named WD4DLL.WAP, which will be discussed later) of the thermal hydrologic and chemistry time history file.

The WAPDEG_External element calls the WAPDEG DLL and is discussed in the next section.

The other elements in the GoldSim implementation (DS_FailureGRF, Combined, WP_FailureGRF, GRF_Functions) are used only to produce graphs of the results stored in the DS_Failure, WP_Failure, and Failure_Opening elements.

6.3.2 WAPDEG-GoldSim Interface Overview

The WAPDEG DLL (called by GoldSim through the WAPDEG_External element) is passed 1040 real numbers (by GoldSim through the WAPDEG_Inputs element). Some of these inputs tell the WAPDEG DLL which degradation models to use, while others are values of degradation model parameters. Note that only real numbers are passed between GoldSim and the WAPDEG DLL. As it was desired for some degradation model parameters to be represented by distributions stored in text files, GoldSim and WAPDEG share a “file index” file, WD4DLL.WAP, the contents of which are shown below:

```
  Line   File Name
1  WDdA22x2p5.cdf
2  WDdA22SR00.cdf
3  WDdTi7Sr00.cdf
4  WDKISCCO.fil
5  WDStressO.fil
6  WDndTi7SR00.cdf
7  WDKISCCM.fil
8  WDStressM.fil
9  WDRHcrit.fil
10 WDdA22x0p5.cdf
11 WDMFDNDO.cdf
12 WDMFDSizeO.cdf
13 WDHLW_high_bin2.ou
14 WDKIinO.fil
15 WDKIinM.fil
16 WDMFDNDM.cdf
17 WDMFDSizeM.cdf
18 WDgA22x2p5.cdf
19 WDgA22SR00.cdf
20 WDgTi7Sr00.cdf
21 WDgA22x0p5.cdf
22 WDiA22x2p5.cdf
```

The line numbers and the column headings are not part of the WD4DLL.WAP file, but are included for clarity. Using the WD4DLL.WAP file, GoldSim and WAPDEG can pass file indices (line numbers in the WD4DLL.WAP file) in place of actual file names. The 1040 real numbers and the contents of the files indentified in the WD4DLL.WAP file are the only inputs to the WAPDEG DLL.

The DS_Failure, WP_Failure, and Failure_Opening elements receive the output from the WAPDEG DLL. The DS_Failure element receives a one dimensional table of drip shield first failure times. The WP_Failure element receives a one dimensional table of waste package first failure times. The format of both of these tables is similar; one column containing the drip shield or waste package first failure times in years (sorted in increasing order) and another column containing the cumulative fraction of waste packages of drip shields failed. The Failure_Opening element receives a two dimensional table containing 33 columns and 300 rows. The column contents are explained in Table 12.

Table 12. Column Contents of the Failure_Opening Element.

Column Number	Contents
1	average number of patch failures (per failed drip shield) on the drip shield top
2	average number of pit failures (per failed drip shield) on the drip shield top
3	average number of crack failures (per failed drip shield) on the drip shield top
4	average number of patch failures (per failed drip shield) on the drip shield side
5	average number of pit failures (per failed drip shield) on the drip shield side
6	average number of crack failures (per failed drip shield) on the drip shield side
7	the cumulative number of first patch failures on the drip shield (top and side)
8	the cumulative number of first pit failures on the drip shield (top and side)
9	the cumulative number of first crack failures on the drip shield (top and side)
10	average number of patch failures (per failed waste package) on the waste package layer 1 top
11	average number of pit failures (per failed waste package) on the waste package layer 1 top
12	average number of crack failures (per failed waste package) on the waste package layer 1 top
13	average number of patch failures (per failed waste package) on the waste package layer 1 side
14	average number of pit failures (per failed waste package) on the waste package layer 1 side
15	average number of crack failures (per failed waste package) on the waste package layer 1 side
16	average number of patch failures (per failed waste package) on the waste package layer 1 bottom
17	average number of pit failures (per failed waste package) on the waste package layer 1 bottom
18	average number of crack failures (per failed waste package) on the waste package layer 1 bottom
19	the cumulative number of first patch failures on the waste package layer 1 (top, side, and bottom)
20	the cumulative number of first pit failures on the waste package layer 1 (top, side, and bottom)
21	the cumulative number of first crack failures on the waste package layer 1 (top, side, and bottom)
22	average number of patch failures (per failed waste package) on the waste package layer 2 top
23	average number of pit failures (per failed waste package) on the waste package layer 2 top
24	average number of crack failures (per failed waste package) on the waste package layer 2 top
25	average number of patch failures (per failed waste package) on the waste package layer 2 side
26	average number of pit failures (per failed waste package) on the waste package layer 2 side
27	average number of crack failures (per failed waste package) on the waste package layer 2 side
28	average number of patch failures (per failed waste package) on the waste package layer 2 bottom
29	average number of pit failures (per failed waste package) on the waste package layer 2 bottom
30	average number of crack failures (per failed waste package) on the waste package layer 2 bottom
31	the cumulative number of first patch failures on the waste package layer 2 (top, side, and bottom)
32	the cumulative number of first pit failures on the waste package layer 2 (top, side, and bottom)
33	the cumulative number of first crack failures on the waste package layer 2 (top, side, and bottom)

Waste package failure (for the purposes of averaging) is defined as any penetration (patch, pit, or crack) of the waste package layer 2 (the pseudo-inner layer in Figure 4). If there are penetrations of layer 1 (the pseudo-outer layer in Figure 4) of a waste package, but no waste container failures (penetrations of layer 2), the number of waste package failues is set to 0.

6.3.3 Drip Shield Design Input

Given a drip shield surface area and patch size, WAPDEG determines the number of patches to be simulated. As discussed in Section 5.1, 500 drip shield patches were assumed to be sufficient to model the variability in drip shield degradation. The results of sensitivity studies such as the one shown in Figure 6, in which the number of drip shield patches was varied using values of 200, 500, and 1,000 patches per drip shield, clearly show that the results of using 500 versus 1,000 drip shield patches are very similar, providing a basis for the assumption.

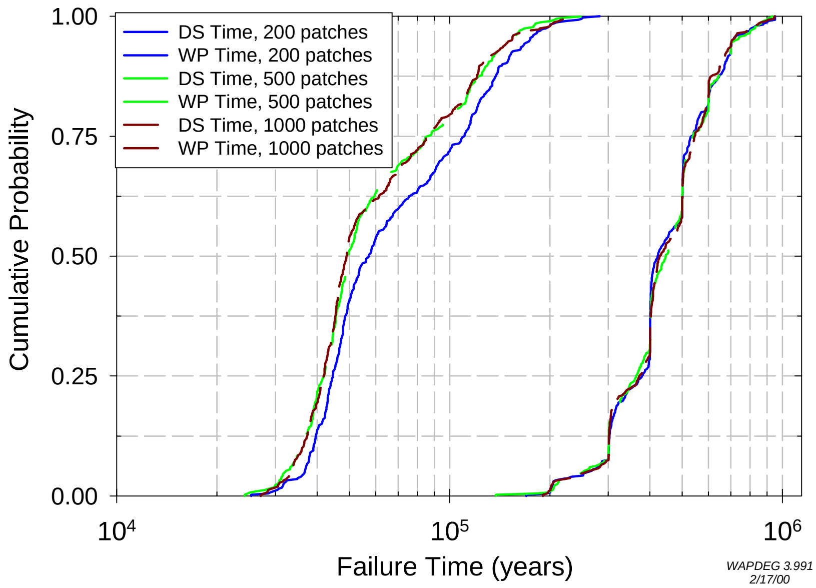

Figure 6. Cumulative Probability of drip shield and waste package failure versus time for simualtions using 200, 500, and 1000 drip shield patches and 400 waste package/drip shield pairs per simulation with 938 waste package patches

6.3.4 Waste Package Design Input

The current waste package design consists of a 20-mm thick Alloy 22 outer barrier encompassing a 50-mm thick 316 NG stainless steel inner barrier (CRWMS M&O 2000n, Section 8.1). No performance credit is taken for the 316 NG stainless steel inner barrier, i.e., the inner barrier is not considered in waste package degradation modeling. The waste package has one Alloy 22 lid on one end of the waste package outer barrier and two Alloy 22 lids (one 10-mm thick inner lid and one 25-mm thick outer lid) on the closure end of the waste package outer barrier. All welds used in waste package fabrication are assumed to be completely stress-annealed with the exception of the closure welds on the two closure lids (see Section 5.5). Thus only the closure lids are subject to stress corrosion cracking. As discussed in Section 6.2, in order to best model the dual Alloy 22 lid design for the waste package outer barrier, the 20-mm Alloy 22 outer barrier is modeled as being composed of two layers; one 25-mm thick and one 10-mm thick. The model parameters (e.g. corrosion rates) are chosen in such a way that the 25-mm thick layer behaves like a 10-mm layer except for the region of that layer that comprises the closure-lid area. For example, the general corrosion rates applied to the 25 mm layer are 2.5 times greater than those for Alloy 22 except for the lid region for which general corrosion rates appropriate for Alloy 22 are used. In the WAPDEG code, waste package failure is defined to be the time of first penetration of the innermost barrier, i.e., the 10-mm inner layer.

Given a waste package surface area and patch size, WAPDEG determines the number of patches to be simulated. As discussed in Section 5.1, 938 waste package patches were determined necessary to achieve computational efficiency. Also in Section 5.1, it was stated that 400 waste package/drip shield pairs were sufficient to model the variability in waste package outer barrier degradation. This conclusion was based on the results of sensitivity studies such as the one shown in Figure 7, in which the number of waste package/drip shield pairs was varied using values of 250 and 500 pairs per simulation. Clearly the results of using 250 versus 500 waste package/drip shield pairs are very similar. The value of 400 pairs was decided upon to allow for computational efficiency and still maintain the ability to capture the variability of the uncertain parameters passed to the WAPDEG DLL.

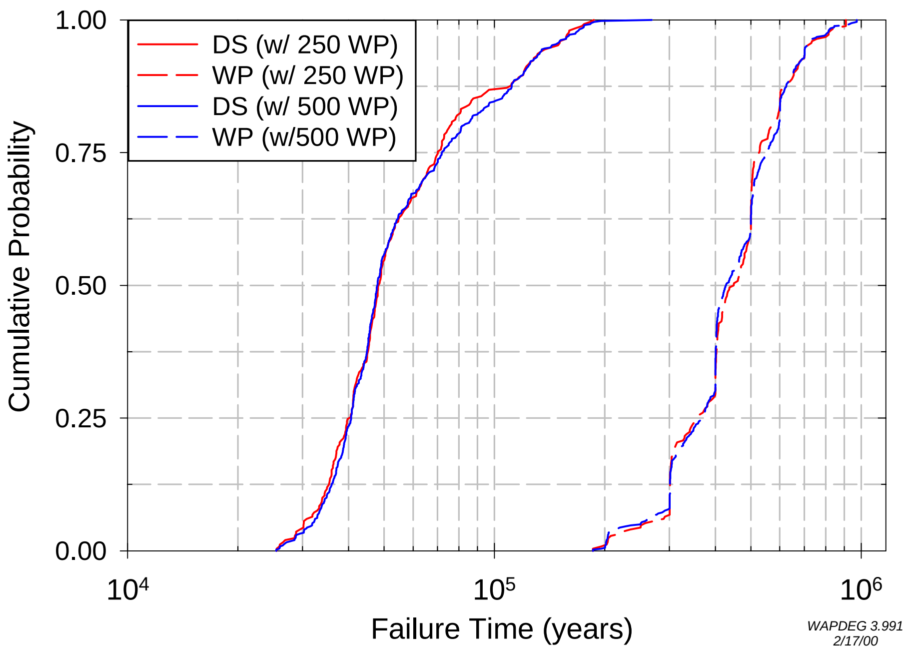

Figure 7. Cumulative Probability of drip shield and waste package failure versus time for simualtions using 250 and 500 waste package/drip shield pairs per simulation with 938 waste package and drip shield patches.

6.3.5 Drip Shield General Corrosion Abstraction Model

6.3.5.1 Drip Shield General Corrosion Abstraction Model Implementation

The rate of general corrosion of the titanium grade 7 drip shield, over the range of thermal-mechanical-chemical repository-relevant exposure conditions, was determined to be insensitive to temperature, stress state, or water chemistry (CRWMS M&O 2000f). In the WAPDEG conceptual model, the water condition above the drip shield could potentially have humid-air conditions followed by dripping water conditions followed by humid-air conditions. The general corrosion rate distribution provided for the drip shield (WDgTi7SR00.cdf) applies to both humid-air and dripping water (aqueous) conditions. However, the variance of the general corrosion rate distribution is due to both uncertainty and variability, which differs for the two conditions. Therefore, two calls are made to the Gaussian Variance Partitioning (GVP) DLL (see Section 6.3.7); one with WDgTi7SR00.cdf as the input and WDdTiSR00.cdf as the output general corrosion rate distribution (used under dripping water conditions), and another with the same WDgTi7SR00.cdf as the input and WDndTiSR00.cdf as the output general corrosion rate distribution (used under humid-air conditions). Details of the GVP implementation are discussed in Section 6.3.7.

6.3.5.2 Drip Shield General Corrosion Abstraction Model Validation

The model validation method used in this section is to observe that the Drip Shield General Corrosion Abstraction Model is derived from qualified experimental data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). The general corrosion rate distribution used (WDgTi7SR00.cdf) was presented in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003. In that calculation, experimentally measured general corrosion rates of Titanium gade 7 (DTN: LL990610605924.079) are sorted in ascending order and assigned cumulative probability values, resulting in the general corrosion rate distribution used in the model. The fact that the general corrosion rate distribution used in the model is derived from qualified experimental data is considered sufficient criteria to validate the model inputs. However, the model is implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason.

6.3.6 Waste Package Outer Barrier General Corrosion Abstraction Model

6.3.6.1 Waste Package Outer Barrier General Corrosion Abstraction Model Implementation

The rate of general corrosion of the Alloy 22 waste package outer barrier, over the range of repository-relevant exposure conditions, was determined to be insensitive to temperature, stress state, or water chemistry (CRWMS M&O 2000e). In the WAPDEG conceptual model, the waste package outer barrier could potentially be contacted by humid-air, dripping, and in-package (inside-out corrosion) water conditions. The general corrosion rate distribution provided for the Alloy 22 waste package outer barrier (WDgA22Sr00.cdf) applies to all these water conditions. As mentioned in Sections 6.2 and 6.3.4, the Alloy 22 waste package outer barrier is modeled as two layers. This necessitated the creation of two additional input cumulative distribution functions (CDFs), both derived from WDgA22SR00.cdf; WDgA22x0p5.cdf in which the general corrosion rates from WDgA22SR00.cdf are multiplied by 0.5 (for inside-out corrosion of the psuedo inner layer) and the cumulative probabilities are left unchanged; and WDgA22x2p5.cdf in which the general corrosion rates are multiplied by 2.5 (for the outside-in corrosion of the pseudo-outer layer) and the cumulative probabilities are left unchanged. Again the variance of the general corrosion rate distributions is due to both uncertainty and variability. Therefore, four calls are made to the Gaussian Variance Partitioning (GVP) DLL; once with WDgA22x2p5.cdf as the input and WDdA22x2p5.cdf as the output general corrosion rate distribution (used under humid-air and dripping conditions for the waste package outer layer), once with WDgA22SR00.cdf as the input and WDdA22SR00.cdf as the output general corrosion rate distribution (used under humid-air and dripping conditions for the waste package inner layer), once with WDgA22x2p5.cdf as the input and WDiA22x2p5.cdf as the output general corrosion rate distribution (used under in package conditions for the waste package outer layer), and once with WDgA22x0p5.cdf as the input and WDdA22x0p5.cdf as the output general corrosion rate distribution (used under in package conditions for the waste package inner layer). As discussed in Section 6.3.2, waste package failure is defined as any penetration (patch, pit, or crack) of the waste package (pseudo) layer 2 (see Figure 4). Therefore, inside-out corrosion of waste package layer 1 (possible only after waste package breach) has no impact on the results of a given WAPDEG simulation. However, input must be provided to the WAPDEG code for all possible degradation mechanisms. Details of the GVP implementation are discussed in Section 6.3.7.

6.3.6.2 Waste Package Outer Barrier General Corrosion Abstraction Model Validation

The model validation method used in this section is to observe that the Waste Package General Corrosion Abstraction Model is derived from qualified experimental data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). The general corrosion rate distribution used (WDgA22SR00.cdf) was presented in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0003SPASUP02.003. In that calculation, experimentally measured general corrosion rates of Alloy 22 (DTN: LL990610605924.079, LL000112205924.112) are sorted in ascending order and assigned cumulative probability values resulting in the general corrosion rate distribution used in the model. The fact that the general corrosion rate distribution used in the model is derived from qualified experimental data is considered sufficient criteria to validate the model inputs. However, the model is implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason.

6.3.7 Gaussian Variance Partitioning

Two containers in the GoldSim implementation have not been discussed; the GVP_External container and the Variance_Shares container. The function of these containers are similar. Gaussian Variance Partitioning (GVP) is a routine that decomposes a cumulative distribution function (CDF) containing both uncertainty and variability into two distributions that characterize each element separately. This is accomplished primarily by partitioning the variance of the original distribution between the two resulting distributions. Gaussian variance partitioning provides a better understanding of the sensitivity of TSPA models to the elements of uncertainty and variability. For further discussion of the GVP algorithm, refer to Attachment I. As shown in Figure 9, the Container GVP_External contains six containers.

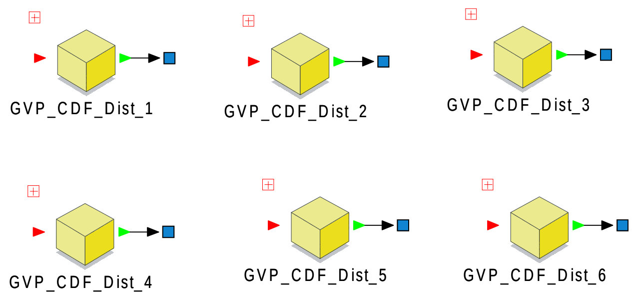

Figure 8. GoldSim implementation which calls the WAPDEG software.

Each of these contains the necessary inputs and parameters for a call to the GVP subroutine. For example, Figure 10 shows the contents of the GVP_CDF_Dist_1 container.

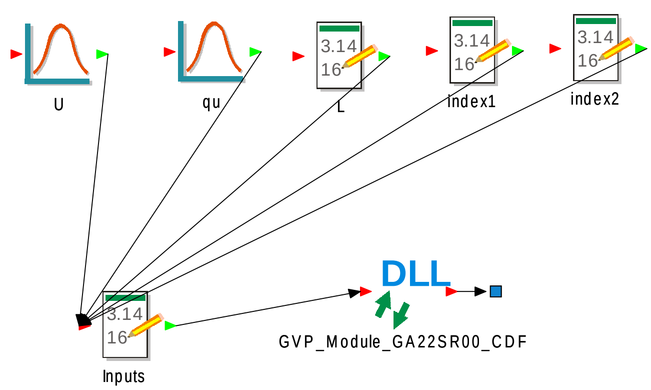

Figure 9. GoldSim implementation which calls the WAPDEG software.

The stochastic element, U, is the uncertain fraction of the original distribution's variance that is due to uncertainty and is sampled from a uniform distribution with bounds of zero and one. The uncertain probability, qu, is used to sample the median of the variability distribution from the uncertainty distribution and is uniformly distributed between zero and one. L is a "flag" used to determine whether the natural logarithm should be taken of the input CDF values (column 1) before GVP operates (and antilogartithms afterward). If L is greater than zero, then logaritms are taken. For all six GVP calls, logarithms of the input values were not taken (L<0). Index1 is the file index (line number in the WD4DLL.wap file) of the input CDF and Index2 is the file index of the output CDF (the partitioned CDF output by the GVP subroutine). These inputs are stacked in a data element named Inputs before being passed to the GVP DLL through the GVP_Module_GA22SR00_CDF element. The other five calls to the GVP DLL are similar, differing only in the file indexes used and the name given to the GVP_Module element.

6.3.8 Relative Humidity Threshold Abstraction Model

6.3.8.1 Relative Humidity Threshold Abstraction Model Implementation

The relative humidity (RH) threshold (WDRHcrit.fil) variance is totally due to variability as no uncertainty treatment was presented in the upstream analysis that supplied this data (CRWMS M&O 2000b, Tables 7 and Figure 8) (also see DTN: LL991212305924.108). For a given WAPDEG realization, the RH threshold distribution is applied as an initiation critieria for all corrosion degradation modes on the drip shield and both of the waste package layers. If the RH read from the exposure file exceeds the critical RH (which is a function of the temperature read from the exposure file), then corrosion degradation can initiate.

The relationship between the critical threshold RH and exposure temperature is given by a lookup table (WDRHcrit.fil), which is listed below:

```
!  WDRHCrit.fil
!
#  1     2
#    19
#    1.0
!  T (°C), RH (frac.)
5         0.7857
10        0.7753
15        0.7646
20        0.7536
25        0.7425
30        0.7314
35        0.7206
40        0.71
45        0.6999
50        0.6904
55        0.6815
60        0.6735
65        0.6664
70        0.6604
75        0.6556
80        0.6522
85        0.6503
90        0.65
120.6     0.501
```

The lines preceded by a "!" are comment lines. The first line preceded by a "#" indicates that there is 1 RH critical relationship with 2 columns. The next line preceded by a "#" indicates that there are 19 rows in the lookup table. The next line preceded by a "#" indicates that this lookup table corresponds to all of the waste packages/drip shields to be simulated (a fraction of 1). This is followed by one more comment line, which is used to specify column headers. The following 19 rows consist of temperature (°C) and RH (fraction) data pairs.

6.3.8.2 Relative Humidity Threshold Abstraction Model Validation

The model validation method used in this Section is to observe that the Relative Humidity Threshold Abstraction Model is derived from accepted experimental data and conservatively assumes the presence of a $NaNO_3$ salt film (see Section 5.2) at all times. This results in an appropriate level of confidence in the model to consider it partially validated (see below). The relative humidity versus temperature data used (WDRHcrit.fil) was presented in an AMR entitled *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000b, Tables 7 and Figure 8) (also see DTN: LL991212305924.108). The fact that the relative humidity versus temperature data used in the model are derived from accepted experimental data and is considered conservative is sufficient criteria to validate the model parameters. However, the model is implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason.

6.3.9 Drip Shield Localized Corrosion Initiation Threshold and Rate Abstraction Model Implementation

As discussed in Section 5.2, there is no localized corrosion initiation threshold or localized corrosion rate model for the drip shield implemented in the WAPDEG conceptual model. As shown in Figure 2 (Section 4.1.6), localized corrosion of titanium grade 7 cannot initiate even at a pH of 14 based on the 3• and 4• confidence intervals.

6.3.10 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

6.3.10.1 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model Implementation

Localized corrosion initiation for the waste package Alloy 22 outer barrier can only occur when the waste package surface is exposed to dripping water (see Section 5.4). During each time step, the WAPDEG DLL evaluates Equation 1 using the pH values read from the exposure file. If evaluation of Equation 1 yields a negative value (i.e., $Ecrit1 < Ecorr$), then localized corrosion can initiate. The rate of localized corrosion is given by the values listed in Table 2 (also see Section 5.3). As indicated by Figure 1 (Section 4.1.5), localized corrosion of Alloy 22 can not initiate at any pH based on the 4• confidence interval.

6.3.10.2 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model Validation

The localized corrosion initiation model used for the Alloy 22 waste package outer barrier is validated in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d) (DTN: MO0003SPAPCC03.004).

The localized corrosion rate portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model is validated by the observation, in Section 5.4, that the localized corrosion rate data is a conservative representation of localized corrosion rate of Alloy 22. This observation provides confidence in the adequacy of the localized corrosion rate model and that it is appropriate for its intended use.

6.3.11 Manufacturing Defect Abstraction Model

6.3.11.1 Manufacturing Defect Abstraction Model Implementation

The MFD_External (in the GoldSim implementation, see Figure 6) consists of two containers as shown in Figure 11.

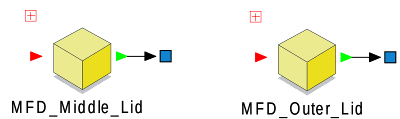

Figure 10. Contents of MFD_External Container in the GoldSim implementation (see Figure 5).

Each of these contains the inputs and parameters necessary to call the MFD subroutine. The contents of the container MFD_Middle_Lid (used to provide input to modeling of the waste package Alloy 22 inner lid) are presented in Figure 12. Note that throughout the GoldSim implementation figures, the Alloy 22 outer barrier inner lid is referred to as the middle lid.

The data element, thickness, is the lid thickness in mm. The outer waste package lid is 25 mm thick while the inner waste package lid is 10 mm thick (CRWMS M&O 2000g) (DTN: MO0001SPASUP03.001). The data element lid_radius is 0.76 m for both the outer and inner waste package lids. The non-detection probability parameters, b and v, uniformly range between 1.6 to 5 mm and 1 to 3 (see Section 4.1.7), respectively. The fraction of waste package surface breaking fractures, psi, is sampled from a uniform distribution with bounding values of 0.0013 and 0.0049 (see Section 4.1.7). The data elements fileFlaws and fileSize are the file indices for the cumulative distribution functions representing the number of manufacturing defect flaws (file index 16) and their lengths (file index 17), respectively. These inputs are passed to the MFD DLL through the MFD_Mod element. The other call to the MFD DLL (contained in the container MFD_OuterLid) is similar, differing only in the file indexes used (11 and 12) and the lid thickness used (25 mm for the waste package outer lid). For further discussion of the MFD algorithm, refer to Attachment II.

All of the data and parameters discussed in this section were documented in the calculation entitled *Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis* (CRWMS M&O 2000g) and are tracked by DTN: MO0001SPASUP03.001.

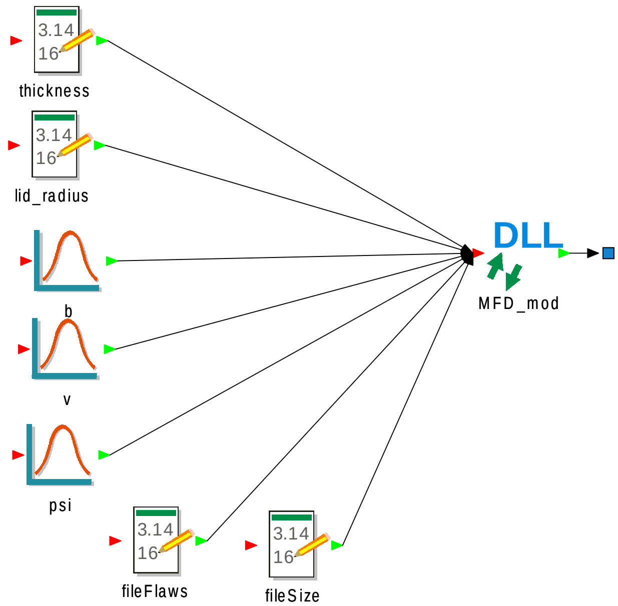

Figure 11. Contents of the MFD_MiddleLid Container in the GoldSim implementation (see Figure 5).

6.3.11.2 Manufacturing Defect Abstraction Model Validation

The model validation method used in this section is to observe that the Manufacturing Defect Abstraction Model parameters derived from qualified developed data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). All of the data and parameters used in this model are documented in the calculation entitled *Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis* (CRWMS M&O 2000g) and are tracked by DTN: MO0001SPASUP03.001. The fact that the parameters used in the model are derived from qualified developed data is considered sufficient criteria to validate the model inputs. However, the model is partially implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason. Attachment II serves as sufficient validation for that portion of the Manufacturing Defect Abstraction Model that is implemented in the MFD DLL.

6.3.12 Stress and Stress Intensity Profile Abstraction Model

6.3.12.1 Stress and Stress Intensity Profile Abstraction Model Implementation

The numerical manipulations discussed in Section 4.1.8 are implemented within the SCCD_External container which is called by the GoldSim implementation (see Figure 6). The contents of the SCCD_External container are shown in Figure 13.

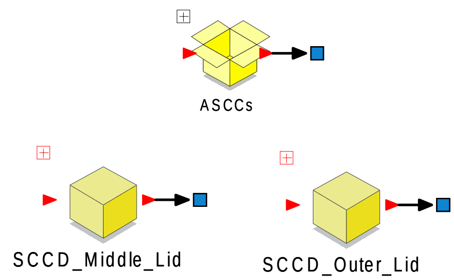

Figure 12. Contents of the SCCD_External Container in the GoldSim implementation (see Figure 5).

The contents of the container SCCD_Middle_Lid are shown in Figure 13. These data elements and functions implement the Stress and Stress Intensity Profile Abstraction discussed in Section 4.1.8 and parts of the Slip Dissolution Model Abstraction discussed in Section 4.1.9. The data element idxinp contains the file index for the input stress intensity (K_I) versus depth profiles listed in Table 6. The data elements A1 through A4 contain the stress coefficients listed in Table 7. The data element amp contains the amplitude of the stress variation used in Equation 6 (*17.236892*). The data element nangle contains the number of angles at which Equation 7 will be evaluated (5 or at each • /5 radians). The data elements YS and fys contain the yield strength and yield strength scaling factor (*F*), respectively, as listed in Table 8. The stochastic element s represents the *z* argument to the *rscale(• ,z)* function shown in Equation 8. *z* is sampled from a truncated normal distribution with a mean of zero, a standard deviation of 1 and upper and lower bounds of –3 and 3, respectively. The data element sinf contains the sine of the angle of projection that the crack path makes with the lid normal. The function Stress_ThreshML expression element takes the output of the Stress_ThreshMLfrac expression element (a value sampled from a unform distribution between 0.2 and 0.3 perfectly correlated to the value sampled for *z*) and multiplies it by the yield strength contained in the YS data element to obtain the stress threshold for propagation of stress corrosion cracks (see Table 9). The data elements idxkin and idxstr contain the file indices for the output K_I and stress variability distributions (7 and 8, respectively). For further discussion of the SCCD algorithm, refer to Attachment III.

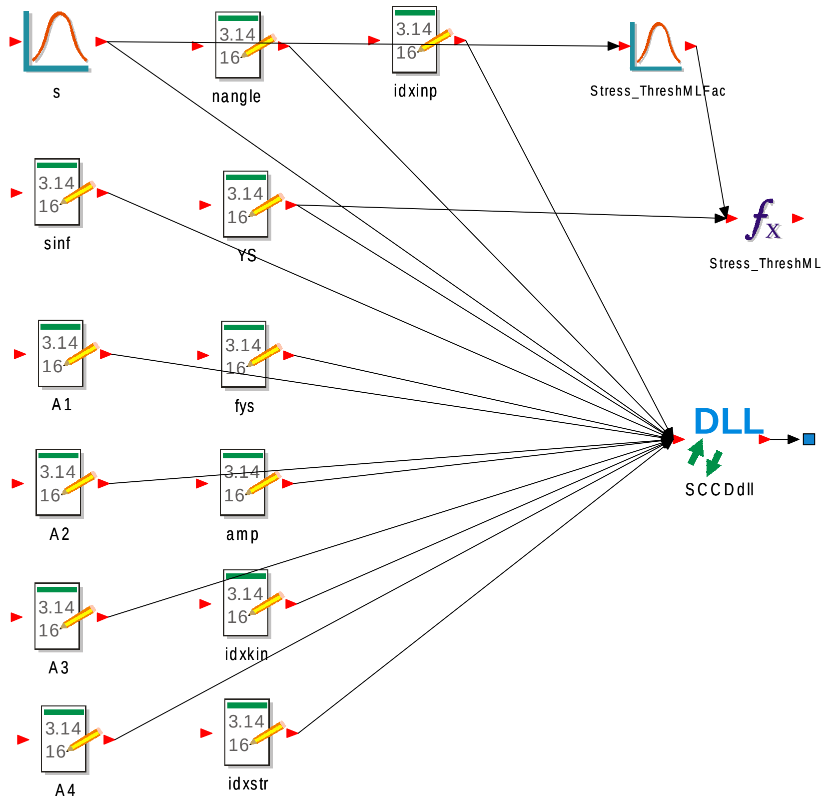

Figure 13. Contents of SCCD_Middle_Lid Container.

6.3.12.2 Stress and Stress Intensity Profile Abstraction Model Validation

The model validation method used in this section is to observe that the Stress and Stress Intensity Profile Abstraction Model parameters are derived from qualified developed data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003. The fact that the parameters used in the model are derived from qualified developed data is considered sufficient criteria to validate the model inputs. However, the model is partially implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason. Attachment III serves as sufficient validation for that portion of the Stress and Stress Intensity Profile Abstraction Model that is implemented in the SCCD DLL.

6.3.13 Slip Dissolution Abstraction Model

6.3.13.1 Slip Dissolution Abstraction Model Implementation

The contents of the ASCCs container (see Figure 12) are shown in Figure 14.

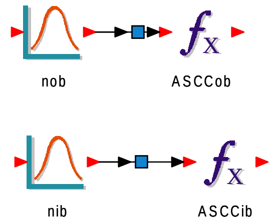

Figure 14. Contents of the ASCCs container in the SCCD_External container (see Figure 12).

The nob and nib stochastic elements sample the value of $\bar{n}$ (see Equation 9) to be used in modeling for the outer and inner lids, respectively. $\bar{n}$ is sampled from a uniform distribution between 3 and 3.36. The expression elements ASCCob and ASCCib use the values of nob and nib (respectively) to evaluate Equation 10 (using Equation 11) for the outer and inner lids, respectively.

6.3.13.2 Slip Dissolution Abstraction Model Validation

The model validation method used in this section is to observe that the Slip Dissolution Abstraction Model parameters are derived from qualified developed data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0004SPASDA04.003. The fact that the parameters used in the model are derived from qualified developed data is considered sufficient criteria to validate the model inputs. However, the model is partially implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason. Attachment III serves as sufficient validation for that portion of the Slip Dissolution Abstraction Model that is implemented in the SCCD DLL.

6.3.14 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model

6.3.14.1 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model Implementation

The Waste Package Outer Barrier MIC Model consists of a threshold relative humidity (RH) and a general corrosion rate multiplier. During each time step, the WAPDEG DLL reads the RH from the exposure file, and if this RH exceeds the threshold RH, MIC is allowed to occur. The effect of MIC is to increase the general corrosion rate by a multiplication factor that is sampled from a uniform distribution with a lower bound of 1 and an upper bound of 2 (see Table 10).

6.3.14.2 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model Validation

The model validation method used in this section is to observe that the Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model parameters are derived from qualified developed data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). All of the parameters used in this model are documented in the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Sections 6.8 and 6.10) and are tracked by DTN: LL991203505924.094. The fact that the parameters used in the model are derived from qualified developed data is considered sufficient criteria to validate the model inputs. However, the model is implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason.

6.3.15 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model

6.3.15.1 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model Implementation

The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model consists of a general corrosion rate multiplier distribution. Upon satisfaction of the relative humidity threshold for initiation of corrosion degradation (Section 6.3.8), the general corrosion rate is enhanced by a multiplier sampled from a uniform distribution with a lower bound of 1 and an upper bound of 2.5 (see Table 11).

6.3.15.2 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model Validation

The model validation method used in this section is to observe that the Waste Package Outer Barrier Aging and Phase Instability Abstraction Model parameters are derived from qualified developed data. This results in an appropriate level of confidence in the model to consider it partially validated (see below). All of the parameters used in this model are documented in the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Sections 6.7.3 and 6.10) and are tracked by DTN: LL000212405924.130. The fact that the parameters used in the model are derived from qualified developed data is considered sufficient criteria to validate the model inputs. However, the model is implemented within the WAPDEG software, which is currently unqualified (see Section 3.1.3), and therefore full validation of the model is not possible for that reason.

6.3.16 Waste Package and Drip Shield Exposure Conditions (RH, T, Drips/No Drips, Seepage Water Chemistry, Etc.)

The exposure condition inputs to the WAPDEG analysis (see Section 4.1.12) are derived from three tables of pH data, two tables of Cl data, and multiple thermo-hydrology infiltration bins containing data on temperature and relative humidity. The PREWAP routine extracts this data from these various tables (DTN: SN0001T0872799.006, MO0002SPALOO46.010, MO9911SPACDP37.001) and prepares an output table that is used as input to the WAPDEG routine. For further discussion of the PREWAP algorithm, refer to Attachment IV.

6.3.17 Variance Sharing

The WAPDEG DLL makes use of several variance sharing parameters. Variance sharing is similar to Gaussian Variance Partitioning between uncertainty and variability. However variance sharing is used to partition the variance of a variability distribution (perhaps resulting from a call to the GVP routine) between waste package to waste package variability and patch to patch variability on a given waste package (and/or crack to crack and pit to pit variability for localized degradation models). That is, given a variability distribution, e.g. a general corrosion cdf, and a variance share, the WAPDEG DLL samples a value for the general corrosion rate for a waste package patch based on the fraction of variance (one of the VarShar_x's).

The contents of the Variance_Share container is shown in Figure 15.

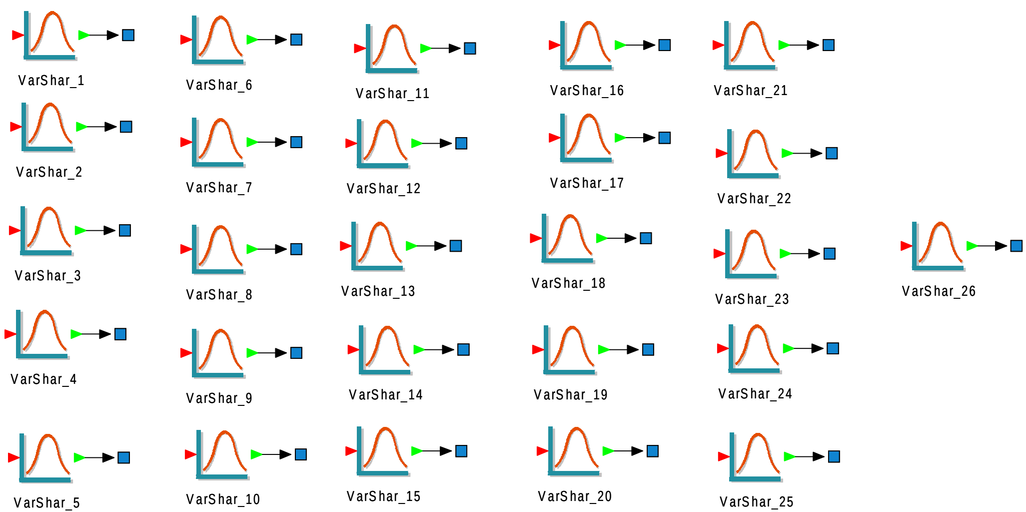

Figure 15. Contents of the Variance_Shares container in the GoldSim implementation (see Figure 5).

Each of the stochastic elements VarShar_1 through VarShar_26 are sampled from a uniform distribution with an upper bound of 1 and a lower bound of zero. These sampled values are used in a similar manner to the stochastic element, U, in the GVP routine discussed in Section 6.3.7.

6.4 ANALYSIS RESULTS

The previous Sections have documented the inputs to the WAPDEG nominal-case analysis. In this section, the results of the WAPDEG nominal-case analysis for waste package and drip shield degradation are presented. As discussed in Section 6.1, the waste package and drip shield degradation analyses to be presented in this Section are for 100 realizations of WAPDEG to account for the uncertainty analysis of the uncertain corrosion parameters. Each WAPDEG realization corresponds to a complete WAPDEG run to represent the degradation variability for a given number of waste package and drip shield pairs. The major simulation parameters used in the analysis are summarized below.

- Temperature, relative humidity, and contacting solution pH histories in the presence of backfill (see Section 6.3.16)
- 400 waste package and drip shield pairs
- 20 mm thick waste package outer barrier (Alloy 22)
- 15 mm thick drip shield (Titanium grade 7)
- 938 patches per waste package
- 500 patches per drip shield

A complete list of input parameters and their values used is given in the input file, bsr8.xls (DTN: MO0004SPASUP01.004). The WAPDEG analysis results (i.e., waste package and drip shield failure time and number of crack, pit and patch penetrations) are reported as a group of “degradation profile curves” that represent the potential range of the output parameters. All input files used in this analysis and output files produced from this analysis are tracked by DTN: MO0004SPASUP01.004. The analysis results are presented for the upper and lower bounds, median, and 95th, 75th, 25th and 5th percentiles as a function of time for the following output parameters:

- Waste package first breach (or failure)
- Drip shield first breach (or failure)
- Waste package first crack penetration
- Waste package first patch penetration
- Waste package crack penetration numbers per failed waste package
- Waste package patch penetration numbers per failed waste package
- Drip shield patch penetration numbers per failed drip shield

Note that localized corrosion does not initiate for either the waste package (Alloy 22 outer barrier) or the drip shield, because the exposure conditions on the drip shield and waste package surface are not severe enough to initiate localized corrosion (i.e., the corrosion potential is less than the threshold corrosion potential) (see Sections 6.3.9 and 6.3.10). Also note that the drip shield is assumed not to be subject to stress corrosion cracking (see Section 6.2), thus no crack penetration failure of the drip shield is calculated. Thus, for the drip shield, the first patch breach time profile is the same as the the failure time profile.

Figure 16 shows the the upper and lower bounds, median, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 51,000 years. Note that the estimated earliest possible first breach time has a very low probability. It can be shown by comparing with the upper bound profile in Figure 19 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration (see the discussion of the results in Figure 17 and Figure 18 later in this Section). The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 120,000 years. The first breach time of the median profile is about 80,000 years. The second waste package breach time of the upper bound and median profiles is about 59,000 and 86,000 years, respectively. The time to fail 10 percent of waste packages for the two profiles is about 80,000 and 171,000 years, respectively.

Figure 17 shows the first breach profiles of drip shields with time. Because the drip shields are not subject to stress corrosion cracking and localized corrosion, the first breach profiles shown in the figure are all by general corrosion only. As discussed in Section 6.2, both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift and are subject to corrosion. In addition, both sides experience the same exposure conditions regardless of whether the drip shields are dripped on or not. Thus, in the analysis, the general corrosion rate for the drip shields is sampled twice independently, once for the patches on the upper side and the once for the patches on the under side. This results in reduced variability in the degradation profiles and thus a fast failure rate (i.e., many drip shields failing over a short time period). This is shown in the upper bound profile, in which the drip shield first breach starts at about 24,000 years and 50 percent of the drip shields fail within a couple of thousand years after the initial failure. Similar trends are also seen with the 95th, 75th and median profiles. In terms of the number of patch penetration openings per failed drip shield with time in Figure 18, the upper bound profile shows that as the drip shields fail, a large number of patches are perforated over a relatively short time period (a few thousand years). A similar trend is seen for the 95th percentile profile. However, the profile shows a larger spread for the other profiles.

Figure 19 and Figure 20 show respectively the first crack penetration and patch penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 51,000 and 61,000 years respectively (Figure 19), and the first patch breach times of the upper and 95th percentile profiles are about 62,000 and 64,000 years, respectively (Figure 20). Comparison of the first crack and patch breach profiles with the first breach profiles in Figure 17 indicates that the initial breach (or failure) of the waste packages is likely by SCC crack penetration in the waste package closure lid welds. For the 75th percentile profiles in the figures, the first crack and patch penetration times are about the same (about 72,000 years). For the remaining profiles, the first crack and patch penetration times are reversed. Therefore, for the median profile, patch breach by general corrosion occurs earlier than crack penetration.

Figure 21 shows the profile for the number of crack penetrations per failed waste package. As discussed for Figure 20, the upper bound and 95th percentile profiles show the first crack penetration at about 51,000 and 61,000 years respectively. For the median profile, the first crack penetration occurrs at about 180,000 years (note the median profile curve starts at about 90,000 years, which has resulted from the interpolation in the post-processing of the WAPDEG analysis results.) Except for the upper bound profile, which represents an extremely low probability condition, the failed waste packages have no more than 5 crack penetrations for up to 100,000 years. SCC cracks in passive alloys such as Alloy 22 tend to be very tight (i.e., small crack opening displacement) by nature (CRWMS M&O 2000a). The opposing sides of through-wall SCC cracks will continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is “plugged” by the corrosion product particles and precipitates such as carbonate present in the water. Any water transport through this oxide/salt filled crack area will be mainly by diffusion-type transport processes(CRWMS M&O 2000a). Thus, both the effective water flow rate into the waste packages and the radionuclide release rate from the waste packages through the SCC cracks would be expected to be extremely low and should not contribute significantly to the overall radionuclide release rate from the repository.

Figure 22 presents the profile for the number of patch openings per failed waste package. For the upper bound profile, which again represents an extremely low probability case, the first patch breach occurs at about 62,000 years (see also Figure 21), and about 100 patches of the failed waste packages (about 10 percent of the waste package surface area) are breached by 100,000 years. In this case, if the waste packages are subject to dripping conditions, the rates of water flow into and radionuclide release from the failed waste packages would be high and thus could affect the repository performance significantly. For the median profile, the first patch opening breach occurs at about 85,000 years, and there will be only two patch openings in each of the failed waste packages by 100,000 years.

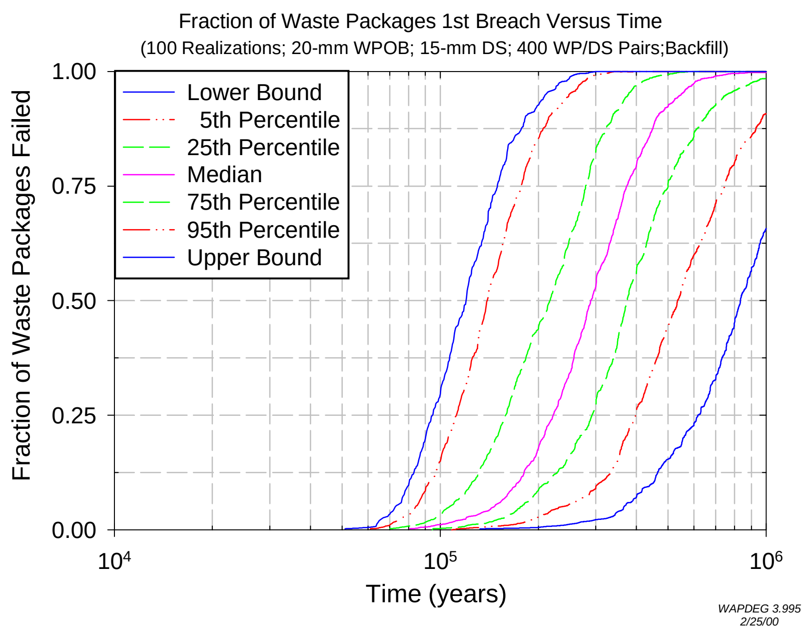

Figure 16. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time.

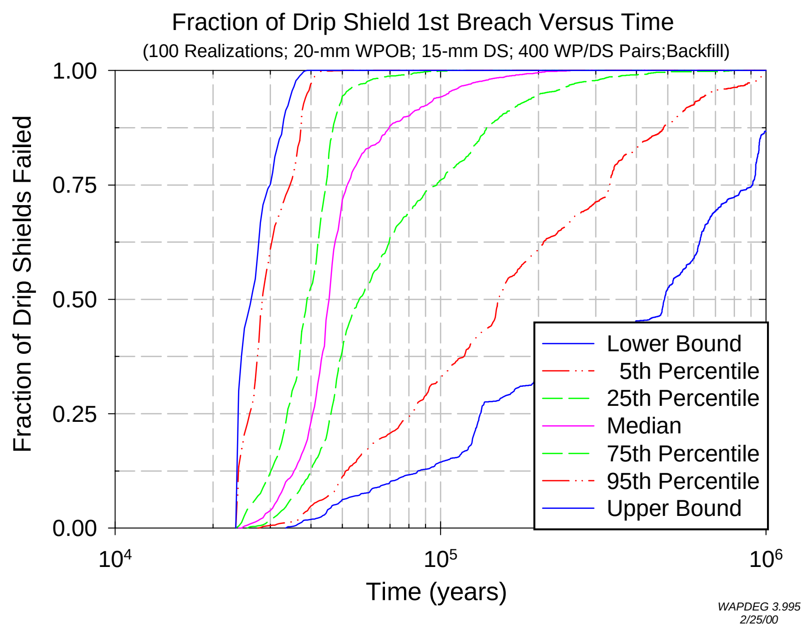

Figure 17. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Drip Shield with Time.

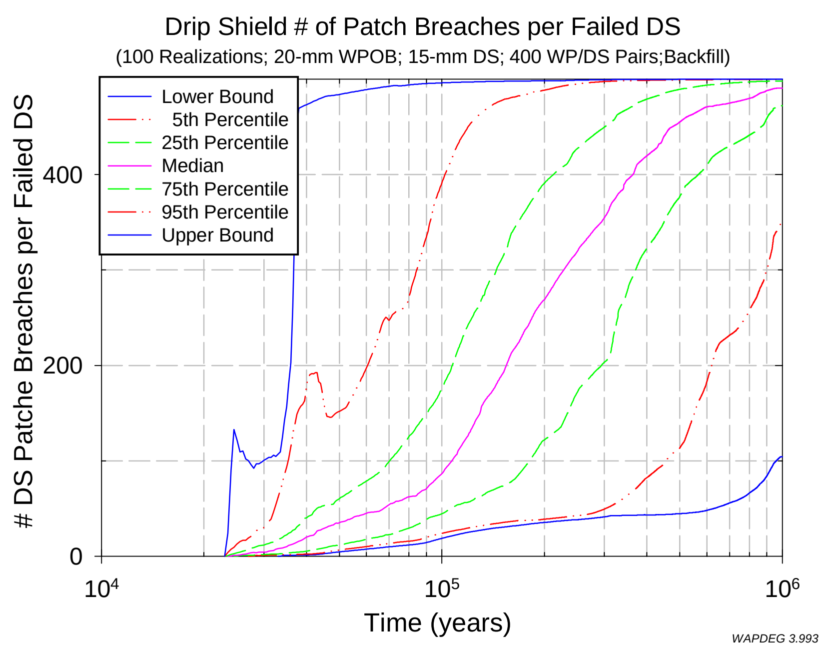

Figure 18. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Number of Patch Penetrations per Failed Drip Shield Profile with Time.

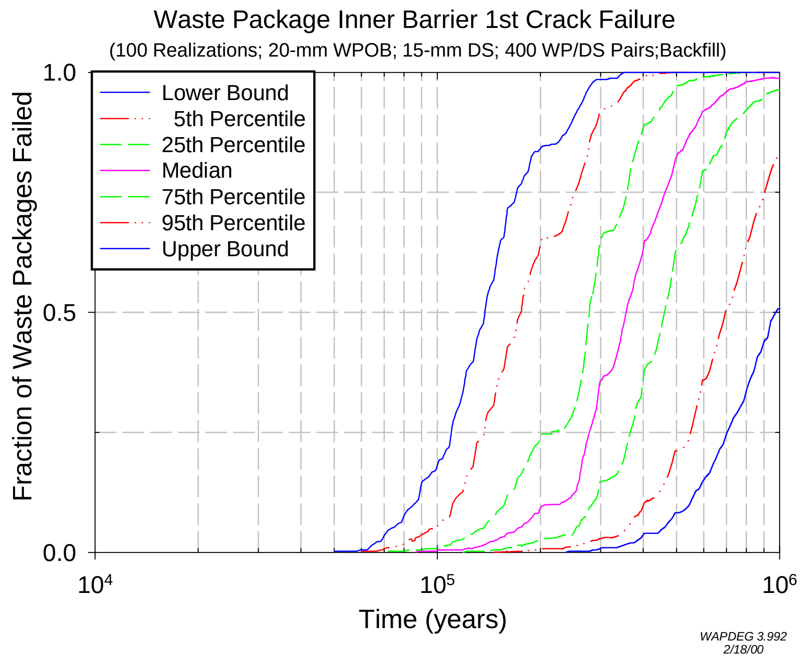

Figure 19. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time.

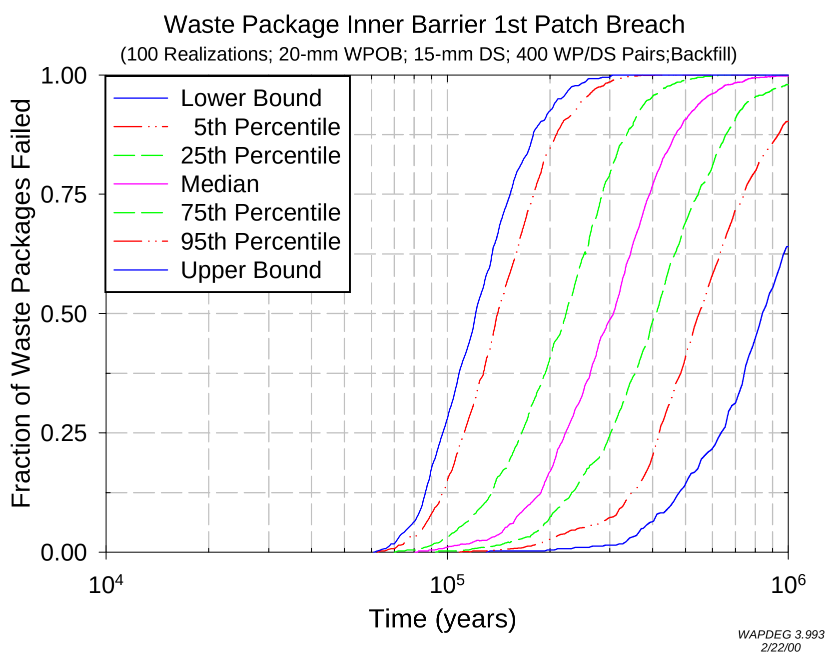

Figure 20. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Patch Breach Profile of Waste Packages with Time.

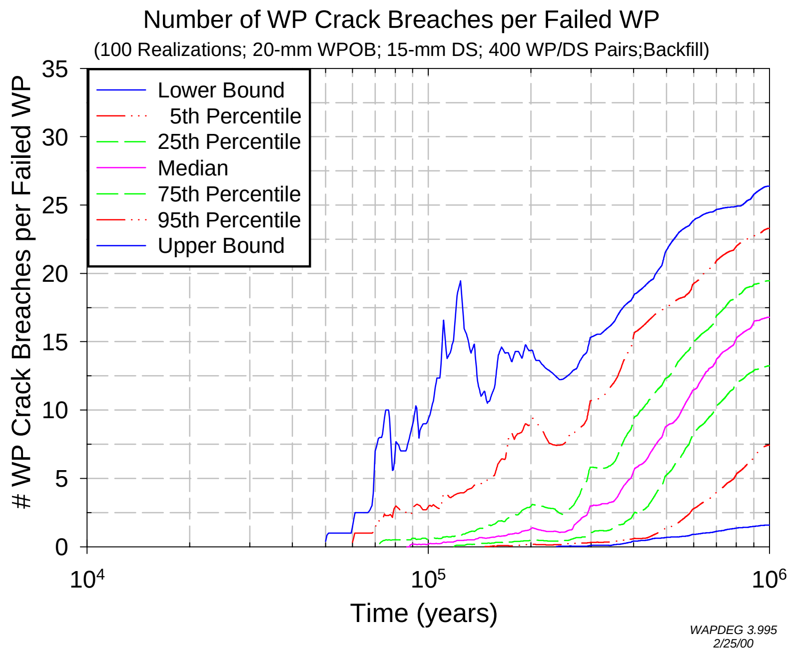

Figure 21. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Number of Crack Penetrations per Failed Waste Package Profile with Time.

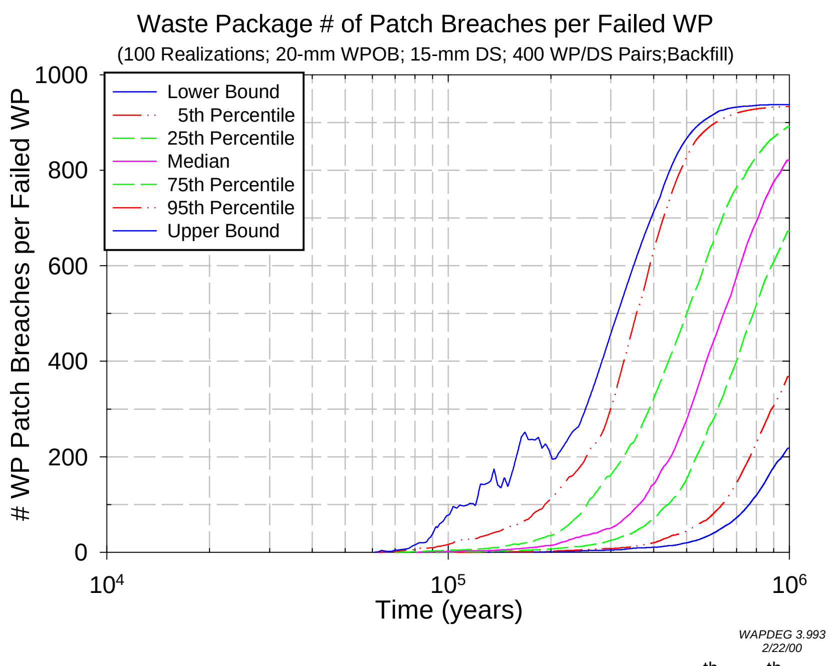

Figure 22. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Number of Patch Penetrations per Failed Waste Package Profile with Time

7. CONCLUSIONS

A conceptual model for the nominal case analysis of degradation of drip shield and waste package in the Yucca Mountain repository was developed, incorporating the data and analyses of the individual degradation processes documented in the companion process-level analysis AMRs (CRWMS M&O 2000a-j, 1999c). The conceptual model and the abstractions of the process-level models and their parameters were incorporated into the integrated waste package degradation model (WAPDEG). Incorporating the exposure conditions (temperature, relative humidity and pH of contacting solution) of the waste packages and drip shields in the repository, the WAPDEG analysis was conducted to develop a detailed description of waste package and drip shield degradation and to develop the degradation abstractions as input to the total system performance assessment (TSPA) analysis.

The waste package and drip shield degradation analyses have shown that based on the current corrosion model abstractions and assumptions, neither the drip shields nor the waste packages fail within the regulatory time period (10,000 years). In particular, the waste package service lifetime is predicted to extend far beyond the regulatory time period (failure beginning at about 50,000 years). The candidate materials for the drip shield (titanium Grade 7) and the waste package outer barrier (Alloy 22) are highly corrosion resistant and, under the repository exposure conditions, are not expected to be subject to the degradation processes that, if initiated, could lead to failure in a short time period. Those degradation modes are localized corrosion (pitting and crevice corrosion), stress corrosion cracking (SCC), and hydrogen induced cracking (HIC) (applicable to drip shield only). Both the drip shield and waste package degrade by general corrosion at very low passive dissolution rates. The current experimental data and detailed process-level analyses, upon which the model abstractions incorporated in the WAPDEG analysis are based, are consistent with this conclusion. Only the closure-lid welds of the waste package, for which complete stress mitigation may not be possible, may be subject to rapidly penetrating corrosion modes under the expected repository conditions (CRWMS M&O 2000e, 2000f, 2000h, and 2000j). Because of the potential residual stresses, the closure-lid welds would be subject to SCC. As discussed in *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i), once a SCC crack initiates, it penetrates the closure-lid thickness in a very short time. The analysis also demonstrated the importance of stress mitigation in the closure-lid welds to avoid premature failures of waste packages by SCC.

To mitigate the SCC threat to potential early failure of the waste package, a dual closure-lid design for the waste package outer barrier has been proposed, and different stress mitigation techniques have been proposed for the dual closure-lid welds: induction heating solution annealing for the outer closure-lid welds and laser peening for the inner closure-lid welds (CRWMS M&O 2000h). The numerical modeling-based analyses have shown that the hoop stress (driving radial cracks) is the dominant stress in the closure-lid welds that could cause SCC failure of waste package. The analyses also have shown that the above stress mitigation techniques can achieve a substantial stress relief for the closure-lid welds (CRWMS M&O 2000h). According to the analyses, mitigation of the hoop stress in the outer closure-lid welds has resulted in a stress state such that the corresponding stress intensity factor for the radial crack is negative to a depth of 12-mm from the surface. For the inner closure-lid welds, the stress intensity factor is negative to a depth of 5-mm. Thus, in the waste package degradation analysis, no SCC cracks initiate in the closure-lid welds until the layer with a negative stress intensity factor (i.e., compressive stress zone layer) is removed by general corrosion.

The predicted long life-time of the waste packages in the current analysis is attributed mostly to 1) the stress mitigation to the substantial depths in the dual closure-lid welds and 2) the very low general-corrosion rate applied to the closure-lid welds to remove the compressive stress zones, providing a long delay time before initiating SCC crack growth. One of the major uncertainties associated with the current analysis is the technical challenge and demonstration to achieve the stress mitigation in the closure-lid welds as dictated from the numerical analyses. In addition, because of a large number of waste packages (12,000 or more) to be emplaced in the repository and because the closure-lid welding will be conducted remotely, the quality control and quality assurance (QC and QA) in the welding and subsequent stress mitigation would be another major uncertainty. The uncertainties associated with the hoop stress and stress intensity factor used in the current analyses need to be closely re-evaluated for the future analysis. Other major uncertainty in the current analysis is the general corrosion rate used for the closure-lid welds. Additional testing and analyses are needed to confirm the general corrosion rate.

Other uncertaities associated with the current analysis have to do with the modeling assumption that the non-closure lid weld area of the waste package is fully annealed and no significant stress state is expected to develop during the life-time in the repository. This assumption will be evaluated as additional data and/or analysis is developed. In addition, there are uncertainties in the current analysis from the use of conservative assumptions. One example is the hoop stress and corresponding (radial crack) stress intensity factor profiles used in the current analysis, which are for the condition at the time of manufacturing. As a crack propagates in the closure-lid welds and/or the welds are thinned by general corrosion, stresses in the welds may re-distribute in such a way that the SCC initiation and crack growth are mitigated (see Section 5.5) (CRWMS M&O 2000h). Such a stress re-distribution or relaxation is not considered in the current abstraction.

Additionally, because of the conservatism in the current threshold RH to initiate corrosion of the drip shield and waste package, no benefit of the drip shield is captured in the WAPDEG analysis for waste package degradation. As discussed in Section 6.2, the threshold RH is based on the deliquescence point of $NaNO_3$ salt as a function of temperature (this effectively incorporates any effect of dust deposition on the waste package surface from any preclosure activities). The same threshold RH is used for both the dripping and non-dripping cases. Realistically, while the drip shield is operative, it will keep the corrosive dripping water from contacting the underlying waste package and provide more benign (or less corrosive) exposure conditions for the waste package. A more realistic model for the corrosion initiation threshold is needed.

Analyses documented in this AMR are limited to the Enhanced Design Alternative (EDA) II and the waste-package outer barrier dual-lid design. The results may not be applicable to other design considerations.

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur, as a result of completing the confirmation activities, will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

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9. ATTACHMENTS

I - GVP Software Routine Report

II - MFD Software Routine Report

III - SCCD Software Routine Report

IV - PREWAP Software Routine Report

ATTACHMENT I

GVP SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Name and Version Number: GVP (Gaussian Variance Partitioning), version 1.01

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 5.0, Standard Edition.

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

2. DESCRIPTION AND TESTING

GVP is a routine that decomposes a Cumulative Distribution Function (CDF) containing both uncertainty and variability into two distributions that characterize each element separately. This provides a better conceptual understanding of TSPA model sensitivity to the elements of uncertainty and variability. The outputs of GVP are:

- A text file containing a CDF table for the variability distribution, and
- An output argument which contains the median of the variability distribution.

2.1 DESCRIPTION OF SOFTWARE ROUTINE AND THE EXECUTION ENVIRONMENT

The GVP source code is a Fortran program 262 lines in length. It conforms to the Fortran 90 standard and is thus highly portable. The subroutine GVP was developed and tested in the Windows NT 4.0 operating system, and has been compiled with Visual Fortran 5.0, Standard Edition for Microsoft Windows 32 bit operating system environments. GVP compiled as a dynamic link library (GVP.DLL) may be coupled with GoldSim (Golder Associates 2000) though its external element mechanism. Inserting data elements in the GoldSim environment allows input parameters to be specified. GVP directly links to and runs within GoldSim for modeling waste package failures. The outputs are used by GoldSim to generate distributions for waste package failures and consequent dose.

The CDF table file formats consists of a first line containing the number of rows in the CDF lookup table with the following lines containing two columns of numbers. The first column of numbers is the distribution values in increasing order. The second column contains the cumulative probability values.

Compilation of GVP requires several Fortran modules to be present from the WAPDEG library (CRWMS M&O 1999f). These are modDefaultSize and modStandardNormal.

The bulk of GVP's coding is devoted to computing the variability distribution by calculation of normal scores. The inputs are read as part of the argument list of GVP, as the elements of array in(*):

in(1) = The fraction of the variance belonging to uncertainty.
in(2) = The fractile value of the uncertainty distribution to place the median value of the variability distribution.
in(3) = Take logarithmic transform (positive value, yes; zero or negative value, no).
in(4) = file index for the input file (combined uncertainty and variability) CDF.
in(5) = file index for the output file (variability) CDF.

The last two inputs are indices (line numbers) within a reference list file (WD4DLL.WAP) for filenames used by several External Functions used by GoldSim for waste package simulation.

The output consists of the variability CDF written to the files indexed in(5), and the median of the variability distribution (written to out(1)). Like all GoldSim External Functions, the coding standard requires all External Functions to accept as input a method variable, which controls the operation of the program. If an External Function is called with the following values of method, the following will occur:

method = 0 Initialize (GVP requires no initialization, thus nothing happens).
method = 1 Normal calculation (for GVP, compute the variability CDF).
method = 2 Report the version number as out(1).
method = 3 Report the number of input and output arguments as out(1) and out(2), respectively (for GVP, this should yield the values 5 and 1, respectively).
method = 99 Clean up, close any open files.

2.2 DESCRIPTION OF THE ALGORITHM

Gaussian variance partitioning starts with a distribution that involves both uncertainty and variability and then works backward to obtain two separate distributions, one that characterizes variability and another that characterizes uncertainty. This is accomplished by assuming that uncertainty and variability are independent. If the mixed distribution is normally distributed, i.e. $N(\mu, \sigma_\mu^2 + \sigma_v^2)$, then it can be represented as a random variable γ having the form

$$\gamma = m + v$$

where m is a normal random variable with mean μ and variance σ_μ^2, and v is a normal random variable with mean zero and variance σ_v^2. Thus, γ is a random variable distributed around the mean μ with a total variance given by the sum of the variances due to uncertainty and variability. If uncertainty is defined as the uncertainty in the mean value and variability as the variance about that mean, then γ can be alternatively parameterized as

$$\gamma \sim N(m,\sigma_v^2), \text{ where } m \sim N(\mu,\sigma_\mu^2)$$

The uncertain mean is represented by the random variable, m, which is normally distributed with mean, μ and variance, σ_μ^2. The random variable, γ, is then the convolution of the distributions of the random variable given by m and a random variable, v, which can be represented by the addition of two normal random variables as given above where

$$m \sim N(\mu,\sigma_\mu^2) \text{ and } v \sim N(0,\sigma_v^2)$$

Thus, given the distributions for m and v, a variability distribution is realized by sampling a value from the parameter uncertainty distribution and adding it to the mean zero variability distribution.

This partitioning method can be extended to non-normal distributions by means of a score transform (Deutsch and Journel 1992, p.138) mapping the percentiles of the non-normal CDF to those of the standard normal by a lookup table. The normal score transforms works best if the non-normal CDF is as symmetric as possible. This may sometimes be accomplished by using the natural logarithms of CDF values. The natural logarithms of the CDF values are used to perform the normal score transformation and the transformed distribution is used to partition the total variance of the transformed distribution between uncertainty and variability. Finally the normal score transformation is applied in reverse to the resultant distributions to obtain a final distribution for variability.

The GVP subroutine was developed to effectively create variability distributions from randomly distributed input data consistent with the above approach.

2.3 DESCRIPTION OF TEST CASE

Industry standard software used to test the GVP routine are:

- MathCad 2000 Professional. This software was used to perform hand calculation verification of GVP

- Excel 97 SR-2. Excel was used to compare the outputs from MathCad and GVP.

The above software programs were executed on an IBM-compatible workstation equipped with a Pentium II processor in the Windows NT operating system

The GVP routine performance was verified by running it in GoldSim and comparing its output to that of a MathCad model using the same CDF as input. Since the inputs used for these calculations are not considered data, they do not require a TBV/TBD tracking number. Three test cases were run to validate the routine across the range of expected inputs. The outputs were imported to an Excel worksheet to compare and quantify the differences. The Excel results for each test case are presented in Tables 1-3.

The MathCad model uses the built-in MathCad functions cnorm, qnorm, and linterp. The MathCad worksheet text is included in Section 3.

The test case requires an input file, a text file WD4DLL.wap, which is a list of filenames to be read by GVP. A listing of WD4DLL.wap is provided in Section 3. Lines in the file contain the names of files used by GVP for the input and output CDFs.

2.4 DESCRIPTION OF TEST RESULTS

The following table's present comparisons between GVP and MathCad outputs using the same input CDF.

Table 1. Test Case 1 Comparison

Output From GVP Ver. 1.01		**MathCad Output**		**Difference**	
27.00		27	2		
1.0000000000E-12	0.0000000000E+00	1.0000000000E-12	0.0000000000E+00	0.0000E+00	0.0000E+00
7.9080728003E-06	3.8461538462E-02	7.9080728003E-06	3.8461538462E-02	-3.0700E-17	0.0000E+00
7.9227282370E-06	7.6923076923E-02	7.9227282370E-06	7.6923076923E-02	4.5799E-17	0.0000E+00
8.9166513808E-06	1.1538461538E-01	8.9166513811E-06	1.1538461538E-01	-3.1120E-16	0.0000E+00
1.5980592034E-05	1.5384615385E-01	1.5980592034E-05	1.5384615385E-01	3.6300E-16	0.0000E+00
1.6075475435E-05	1.9230769231E-01	1.6075475435E-05	1.9230769231E-01	-7.2997E-17	0.0000E+00
1.6460828662E-05	2.3076923077E-01	1.6460828662E-05	2.3076923077E-01	4.6800E-16	0.0000E+00
1.9234298278E-05	2.6923076923E-01	1.9234298278E-05	2.6923076923E-01	5.7998E-17	0.0000E+00
2.1997414128E-05	3.0769230769E-01	2.1997414128E-05	3.0769230769E-01	-2.9000E-16	0.0000E+00
2.3587950691E-05	3.4615384615E-01	2.3587950691E-05	3.4615384615E-01	4.5200E-16	0.0000E+00
2.3707715534E-05	3.8461538462E-01	2.3707715534E-05	3.8461538462E-01	-2.5800E-16	0.0000E+00
2.3905721918E-05	4.2307692308E-01	2.3905721918E-05	4.2307692308E-01	-3.1200E-16	0.0000E+00
2.4390559388E-05	4.6153846154E-01	2.4390559388E-05	4.6153846154E-01	-3.7700E-16	0.0000E+00
2.5278489449E-05	5.0000000000E-01	2.5278489449E-05	5.0000000000E-01	-4.3000E-16	0.0000E+00
3.4976429294E-05	5.3846153846E-01	3.4976429294E-05	5.3846153846E-01	-3.2100E-16	0.0000E+00
4.1075553863E-05	5.7692307692E-01	4.1075553863E-05	5.7692307692E-01	4.8600E-16	0.0000E+00
4.2653925254E-05	6.1538461538E-01	4.2653925254E-05	6.1538461538E-01	-1.2100E-16	0.0000E+00
4.2831705762E-05	6.5384615385E-01	4.2831705762E-05	6.5384615385E-01	-2.2200E-16	0.0000E+00
4.7949103820E-05	6.9230769231E-01	4.7949103820E-05	6.9230769231E-01	-2.4002E-17	0.0000E+00
5.5667093052E-05	7.3076923077E-01	5.5667093052E-05	7.3076923077E-01	-4.5900E-16	-9.9920E-16
6.3631129194E-05	7.6923076923E-01	6.3631129194E-05	7.6923076923E-01	2.6099E-16	0.0000E+00
6.4961801788E-05	8.0769230769E-01	6.4961801788E-05	8.0769230769E-01	-3.8500E-16	0.0000E+00
7.0683238187E-05	8.4615384615E-01	7.0683238187E-05	8.4615384615E-01	2.9401E-16	0.0000E+00
7.7898693790E-05	8.8461538462E-01	7.7898693789E-05	8.8461538462E-01	6.5600E-16	0.0000E+00
8.1978768245E-05	9.2307692308E-01	8.1978768244E-05	9.2307692308E-01	6.0000E-16	0.0000E+00
1.1187640145E-04	9.6153846154E-01	1.1187640145E-04	9.6153846154E-01	5.9997E-17	0.0000E+00
3.2500000000E-04	1.0000000000E+00	3.2500000000E-04	1.0000000000E+00	0.0000E+00	0.0000E+00

Table 2. Test Case 2 Comparison

Output from GVP version 1.01		**MathCad Output**		**Difference**	
27.00		27.00	2.00		
1.0000000000E-12	0.0000000000E+00	1.0000000000E-12	0.0000000000E+00	0.0000E+00	0.0000E+00
7.9080729562E-06	3.8461538462E-02	7.9080729562E-06	3.8461538462E-02	-1.4500E-17	0.0000E+00
7.9227517980E-06	7.6923076923E-02	7.9227517980E-06	7.6923076923E-02	-3.9800E-17	0.0000E+00
9.2535733347E-06	1.1538461538E-01	9.2535733351E-06	1.1538461538E-01	-3.8870E-16	0.0000E+00
1.5980628924E-05	1.5384615385E-01	1.5980628924E-05	1.5384615385E-01	-1.1000E-16	0.0000E+00
1.6075496082E-05	1.9230769231E-01	1.6075496082E-05	1.9230769231E-01	3.3300E-16	0.0000E+00
1.6461749708E-05	2.3076923077E-01	1.6461749708E-05	2.3076923077E-01	1.7600E-16	0.0000E+00
1.9362461435E-05	2.6923076923E-01	1.9362461435E-05	2.6923076923E-01	-1.0998E-17	0.0000E+00
2.2031225218E-05	3.0769230769E-01	2.2031225218E-05	3.0769230769E-01	-7.0998E-17	0.0000E+00
2.3588017360E-05	3.4615384615E-01	2.3588017360E-05	3.4615384615E-01	2.8500E-16	0.0000E+00
2.3707782923E-05	3.8461538462E-01	2.3707782923E-05	3.8461538462E-01	2.2999E-17	0.0000E+00
2.3906188955E-05	4.2307692308E-01	2.3906188955E-05	4.2307692308E-01	3.0002E-17	0.0000E+00
2.4397046701E-05	4.6153846154E-01	2.4397046701E-05	4.6153846154E-01	1.9300E-16	0.0000E+00
2.5278489449E-05	5.0000000000E-01	2.5278489449E-05	5.0000000000E-01	-4.3000E-16	0.0000E+00
3.5694618764E-05	5.3846153846E-01	3.5694618764E-05	5.3846153846E-01	-1.0500E-16	0.0000E+00
4.1095792129E-05	5.7692307692E-01	4.1095792129E-05	5.7692307692E-01	3.0200E-16	0.0000E+00
4.2654007281E-05	6.1538461538E-01	4.2654007281E-05	6.1538461538E-01	3.4100E-16	0.0000E+00
4.2831787163E-05	6.5384615385E-01	4.2831787163E-05	6.5384615385E-01	1.9900E-16	0.0000E+00
4.8140240689E-05	6.9230769231E-01	4.8140240689E-05	6.9230769231E-01	-4.1900E-16	0.0000E+00
5.5950749656E-05	7.3076923077E-01	5.5950749656E-05	7.3076923077E-01	2.6001E-17	-9.9920E-16
6.3633879490E-05	7.6923076923E-01	6.3633879490E-05	7.6923076923E-01	-2.5601E-16	0.0000E+00
6.4961864359E-05	8.0769230769E-01	6.4961864359E-05	8.0769230769E-01	-1.6400E-16	0.0000E+00
7.0716507075E-05	8.4615384615E-01	7.0716507075E-05	8.4615384615E-01	-3.0087E-18	0.0000E+00
7.7951300826E-05	8.8461538462E-01	7.7951300826E-05	8.8461538462E-01	-1.1499E-16	0.0000E+00
8.1982636492E-05	9.2307692308E-01	8.1982636491E-05	9.2307692308E-01	5.4301E-16	0.0000E+00
1.1187767631E-04	9.6153846154E-01	1.1187767631E-04	9.6153846154E-01	-2.5400E-15	0.0000E+00
3.2500000000E-04	1.0000000000E+00	3.2500000000E-04	1.0000000000E+00	0.0000E+00	0.0000E+00

Table 3. Test Case 3 Comparison

Output from GVP version 1.01		**MathCad Output**		**Difference**	
27.00		27.0	2.0		
1.0000000000E-12	0.0000000000E+00	1.0000000000E-12	0.0000000000E+00	0.0000E+00	0.0000E+00
6.3582282761E-11	3.8461538462E-02	6.3582282743E-11	3.8461538462E-02	1.7910E-20	0.0000E+00
6.3446588157E-10	7.6923076923E-02	6.3446588137E-10	7.6923076923E-02	2.0251E-19	0.0000E+00
5.0326740107E-09	1.1538461538E-01	5.0326740085E-09	1.1538461538E-01	2.1753E-18	0.0000E+00
3.6855544470E-08	1.5384615385E-01	3.6855544450E-08	1.5384615385E-01	1.9729E-17	0.0000E+00
2.6487663977E-07	1.9230769231E-01	2.6487663953E-07	1.9230769231E-01	2.4123E-16	0.0000E+00
1.9342192774E-06	2.3076923077E-01	1.9342192757E-06	2.3076923077E-01	1.7324E-15	0.0000E+00
4.4095920679E-06	2.6923076923E-01	4.4095920678E-06	2.6923076923E-01	1.4480E-16	0.0000E+00
4.8110822300E-06	3.0769230769E-01	4.8110822298E-06	3.0769230769E-01	1.8540E-16	0.0000E+00
5.2662267575E-06	3.4615384615E-01	5.2662267573E-06	3.4615384615E-01	2.2480E-16	0.0000E+00
5.7875359227E-06	3.8461538462E-01	5.7875359224E-06	3.8461538462E-01	2.9230E-16	0.0000E+00
6.3910264402E-06	4.2307692308E-01	6.3910264399E-06	4.2307692308E-01	2.9670E-16	0.0000E+00
7.0976697807E-06	4.6153846154E-01	7.0976697803E-06	4.6153846154E-01	3.5060E-16	0.0000E+00
7.9054224445E-06	5.0000000000E-01	7.9054224445E-06	5.0000000000E-01	-1.7700E-17	0.0000E+00

Output from GVP version 1.01		MathCad Output		Difference	
7.9060976482E-06	5.3846153846E-01	7.9060976482E-06	5.3846153846E-01	-1.5801E-17	0.0000E+00
7.9068263259E-06	5.7692307692E-01	7.9068263259E-06	5.7692307692E-01	3.5501E-17	0.0000E+00
7.9076192799E-06	6.1538461538E-01	7.9076192799E-06	6.1538461538E-01	3.5901E-17	0.0000E+00
7.9084905343E-06	6.5384615385E-01	7.9084905343E-06	6.5384615385E-01	2.2900E-17	0.0000E+00
7.9100698220E-06	6.9230769231E-01	7.9100698220E-06	6.9230769231E-01	-1.6700E-17	0.0000E+00
7.9126008365E-06	7.3076923077E-01	7.9126008365E-06	7.3076923077E-01	-6.1003E-18	-9.9920E-16
7.9155056342E-06	7.6923076923E-01	7.9155056342E-06	7.6923076923E-01	3.4600E-17	0.0000E+00
7.9314566958E-06	8.0769230769E-01	7.9314566958E-06	8.0769230769E-01	2.9201E-17	0.0000E+00
7.9685378684E-06	8.4615384615E-01	7.9685378684E-06	8.4615384615E-01	4.7400E-17	0.0000E+00
9.9711015058E-06	8.8461538462E-01	9.9711015043E-06	8.8461538462E-01	1.5179E-15	0.0000E+00
1.5988963043E-05	9.2307692308E-01	1.5988963043E-05	9.2307692308E-01	-2.7300E-16	0.0000E+00
1.6378897834E-05	9.6153846154E-01	1.6378897834E-05	9.6153846154E-01	-2.7300E-16	0.0000E+00
3.2500000000E-04	1.0000000000E+00	3.2500000000E-04	1.0000000000E+00	0.0000E+00	0.0000E+00

2.5 RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED

The input data used in the test case covers the range of values from 10^{-12} to $>10^{-4}$. The effective range of the test case covers values ranging from 10^{-6} to $>10^{-4}$, or two decades. No variance between test case values at the smallest value (10^{-12}) and the largest value ($>10^{-4}$) is expected because the probability of the CDF at these endpoints is zero at the low end and 1 at the high end.

From the above tables it is concluded the GVP routine is verified by hand calculation to nine digits over the range of inputs used. This range bounds the data inputs for which the routine will be used.

2.6 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

None.

3. SUPPORTING INFORMATION

3.1 DIRECTORY LISTING OF EXECUTABLES AND DATA FILES

```
Directory of gvptest

02/27/00  03:23p               32,576 gvp.gsm
01/18/00  05:29p               34,882 GVP.mcd
01/27/00  02:51p               28,672 gvp_dll.dll
02/27/00  03:17p                   58 WD4DLL.wap
01/17/00  05:42p                1,456 gTi7SR00.cdf
02/27/00  03:05p                1,456 gTiM5050.cdf
02/27/00  03:18p                1,463 gTiM5050.txt
02/27/00  03:05p                1,456 gTiM7505.cdf
02/27/00  03:22p                1,463 gTiM7505.txt
02/27/00  03:05p                1,456 gTiN5050.cdf
02/27/00  03:19p                1,463 gTiN5050.txt
```

3.2 COMPUTER LISTING OF SOURCE CODE

```
SUBROUTINE gvp(method, state, in, out)
!
!  Subroutine to perform Gaussian Variance Partitioning.
!
!  1. Read combined cdf from an input file, the uncertainty
!     variance share, and the uncertainty quantile level.
!  2. Find/print the variability cdf.
!  Note if log transform option is used the user is responsible
!  for values being in the proper range for the log function.
!
!DEC$ ATTRIBUTES dllexport,c :: gvp
!DEC$ ATTRIBUTES value       :: method
!DEC$ ATTRIBUTES reference   :: state
!DEC$ ATTRIBUTES reference   :: in
!DEC$ ATTRIBUTES reference   :: out
      USE ModDefaultsize
      USE ModStandardNormal
      IMPLICIT NONE
      integer(IKind) :: method   ! input, tells gvp what to do
      integer(IKind) :: state    ! return, 0 = OK
      real(RKind)    :: in(*)    ! input arguments
      real(RKind)    :: out(*)   ! output arguments
      real(RKind), PARAMETER :: VERSION = 1.01
      integer(IKind), PARAMETER :: NUMIN = 5, NUMOUT = 1
      integer(IKind) :: cdfunit , filunit, errunit
      integer(IKind) :: i, n, n1, n2, idxinp, idxout
      real(RKind)    :: U, qu, lntrns, V, zu, medv
      character(LEN = 80) :: inputcdf, outputcdf, line1
      real(RKind), ALLOCATABLE, DIMENSION(:) :: vals
      real(RKind), ALLOCATABLE, DIMENSION(:) :: pvals
      real(RKind), ALLOCATABLE, DIMENSION(:) :: zv
      real(RKind), ALLOCATABLE, DIMENSION(:) :: xv
      logical(LKind) :: OK
!
!**********************************************************************
!
      if (method .eq. 0) then        ! Initialize
        state = 0
        return
      elseif (method .eq. 2) then    ! Report code version
        out(1) = VERSION
        state = 0
        return
```

```
      elseif (method .eq. 3) then    ! Report number of arguments
        out(1) = NUMIN
        out(2) = NUMOUT
        state = 0
        return
      elseif (method .eq. 1) then    ! Calculate
        U  = in(1)
        qu = in(2)
        lntrns = in(3)
        idxinp = in(4)
        idxout = in(5)
!
!  Read I/O CDF-File names from master list file
!
        filunit = nextfreeunit()
        open(unit = filunit, file = 'WD4DLL.WAP')
        n = max(idxinp, idxout)
        do i = 1, n
          read(filunit,*) line1
          if (i .eq. idxinp) inputcdf  = line1
          if (i .eq. idxout) outputcdf = line1
        end do
        close(unit = filunit)
!
!  Open Input CDF-File and read contents
!
        inquire(file = inputcdf, exist = OK)
        if (.not. OK) then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit,file = 'gvperror.log')
          write(errunit,*) 'input file not found'
          close(unit = errunit)
          return
        end if
        cdfunit = nextfreeunit()
        open(unit = cdfunit, file = inputcdf)
        read(cdfunit, *) n
        ALLOCATE(vals(n))
        ALLOCATE(pvals(n))
        ALLOCATE(zv(n))
        ALLOCATE(xv(n))
        do i = 1, n
          read(cdfunit,*) vals(i), pvals(i)
        end do
        close(unit = cdfunit)
!
!  Perform Calculations
!  If log transformed (lntrns) then take logs
!
        if (lntrns .gt. 0.0) then
          do i = 1, n
            vals(i) = log(vals(i))
          end do
        endif
!
!  Check for limits of normal functions
!
        n1 = 1
        n2 = n
        do while (pvals(n1) .le. 1.0D-15)
          xv(n1) = vals(n1)
          n1 = n1 + 1
        end do
        do while (pvals(n2) .ge. (1.0-1.0D-15))
          xv(n2) = vals(n2)
          n2 = n2-1
        end do
!
!  calculate normal values for variability and map back
!  to distribution
```

```
!
        V = 1-U
        zu = sqrt(U)*InvNor(qu)
        medv = linterp1(n,pvals,vals,FwdNorm(zu))
        do i = n1, n2
          zv(i) = zu + sqrt(V)*InvNor(pvals(i))
          xv(i) = linterp1(n,pvals,vals,FwdNorm(zv(i)))
        end do
!
!  If log transformed then take antilogs
!
        if (lntrns .gt. 0.0) then
          medv = exp(medv)
          do i = 1, n
            xv(i) = exp(xv(i))
          end do
        endif
!
!  Output results and clean up
!
        out(1) = medv
        cdfunit = nextfreeunit()
        open(unit = cdfunit, file = outputcdf)
        write(cdfunit,*) n
        do i = 1, n
          write(cdfunit,3332) xv(i), pvals(i)
 3332     format(1x,1pe17.10,2x,e22.15)
        end do
        write(cdfunit,*)
        write(cdfunit,3330) VERSION
        write(cdfunit,3331) U, qu
        write(cdfunit,3338) ( i, in(i), i = 1, NUMIN )
        write(cdfunit,*)
 3330   format('! Output from gvp version ',f4.2)
 3331   format('! Sampled random variables U =',f9.5,',qu =',f9.5)
 3338   format('! argument in(',I2,') = ',f12.5)
        close(unit = cdfunit)
        DEALLOCATE(vals, pvals, zv, xv)
        state = 0
        return
      elseif (method .eq. 99) then   ! Shut-down
        close(unit = filunit)
        close(unit = cdfunit)
        close(unit = errunit)
        state = 0
        return
      else
        errunit = nextfreeunit()
        open(unit = errunit, file = 'gvperror.log')
        write(errunit,*) 'gvp-DLL crashed method = ',method
        close(unit = errunit)
        state = 1
        return
      end if                         ! end block for method
      CONTAINS    ! linterp1, nextfreeunit
!
!**********************************************************************
!
      real(RKind) FUNCTION linterp1(n, x, y, xval)
!
!    linear interpolation routine from a lookup table.
!    Input : n, x, y, xval
!    Output: (function value)
!    Local : i, ii
!
!    Arguments
!
      integer(IKind) :: n
      real(RKind)    :: x(*), y(*), xval
!
!    Local variable
```

```
!
      integer(IKind) :: i, ii
!
      if (xval .le. x(1)) then
        linterp1 = y(1)
      else if (xval .ge. x(n)) then
        linterp1 = y(n)
      else
        ii = 2
        do while (xval .gt. x(ii))
          ii = ii+1
        end do
        i = ii-1
        linterp1 = y(i) + (y(ii)-y(i))*(xval - x(i))/(x(ii)-x(i))
      end if
      RETURN
      END FUNCTION linterp1
!
!**********************************************************************
!
      integer(IKind) FUNCTION nextfreeunit()
!
!  Find the smallest unit number not currently attached and in use.
!  Avoid units 5 and 6.
!  Input : (none)
!  Output: (function value)
!  Local : i, InUse
!
!  Local variables
!
      integer(IKind) :: i
      logical InUse
!
      InUse = .true.
      i = 0
      do while (InUse)
        i = i + 1
        if(i .ne. 5 .and. i .ne. 6) then
          inquire(i, opened = InUse)
        end if
      end do
      nextfreeunit = i
      RETURN
      END FUNCTION nextfreeunit
!
!**********************************************************************
!
      END SUBROUTINE gvp
```

3.3 LISTING OF MATHCAD WORKSHEET

The function, $GVP(p, x, U, qu, lntrns)$, below partitions the variance of the discrete univariate distribution given by the cdf table of values in x and cumulative probabilities in p. By matching probability values we create a table of standard normal score values matched with x values. This table is then used to lookup rate values that correspond to the Gaussian variance partitioning of the standard normal for the given uncertain variability (U) and quantile (qu) both expressed as fractions. Lntrns is an argument used as a programming flag. If lntrns > 0, the values in x are natural logarithm transformed before interpolation (producing semi-log interpolation) and the results of interpolation are exponentiated.

- V is the fraction of the variance that represents variability.
- zu is the standard normal score value that corresponds to the given quantile.

- Values of p and x (or lnx) make up the lookup table.
- The probability values zero and one are mapped specifically to remove the appearances of infinity.
- zv are the standard normal values with mean zu and variance V that corresponds to the variability distribution.
- GVP returns a matrix of values and cumulative probabilities for the variability distribution.

The Mathcad listing of the GVP function is shown below:

$$
\mathrm{GVP}(p, x, U, qu, lntrns) := \left|
\begin{array}{l}
V \leftarrow 1 - U \\
zu \leftarrow \sqrt{U} \cdot \mathrm{qnorm}(qu, 0, 1) \\
lnx \leftarrow \ln(x) \quad \text{if } (lntrns > 0) \\
\text{for } i \in 0 .. \mathrm{length}(x) - 1 \\
\quad \left| \begin{array}{l}
zv_i \leftarrow \left| \begin{array}{ll}
-\infty & \text{if } p_i = 0 \\
\infty & \text{if } p_i = 1 \\
\left(zu + \sqrt{V} \cdot \mathrm{qnorm}(p_i, 0, 1)\right) & \text{otherwise}
\end{array} \right. \\
xv_i \leftarrow \exp\left(\mathrm{linterp}\left(p, lnx, \mathrm{cnorm}(zv_i)\right)\right) \quad \text{if } (lntrns > 0) \\
xv_i \leftarrow \mathrm{linterp}\left(p, x, \mathrm{cnorm}(zv_i)\right) \quad \text{otherwise}
\end{array} \right. \\
\mathrm{augment}(xv, p)
\end{array}
\right.
$$

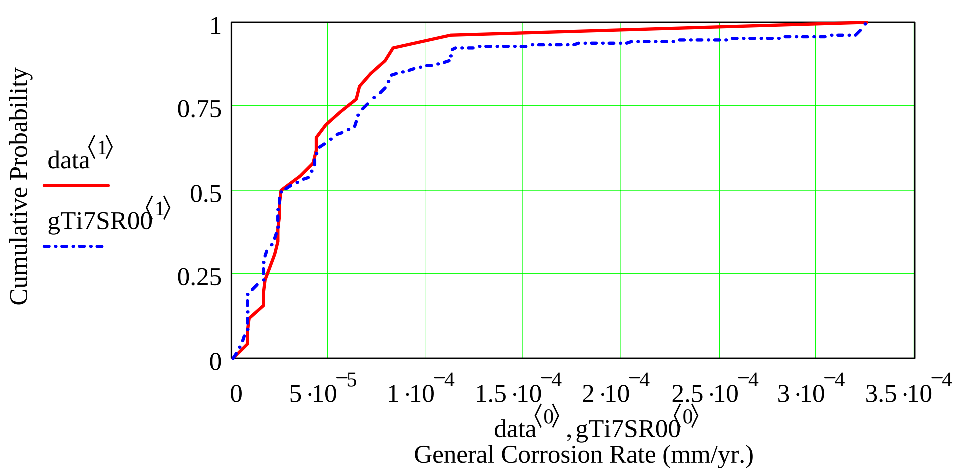
Below is the input CDF data, column 1 contain values, column 2 contain cumulative probabilities.

gTi7SR00 :=

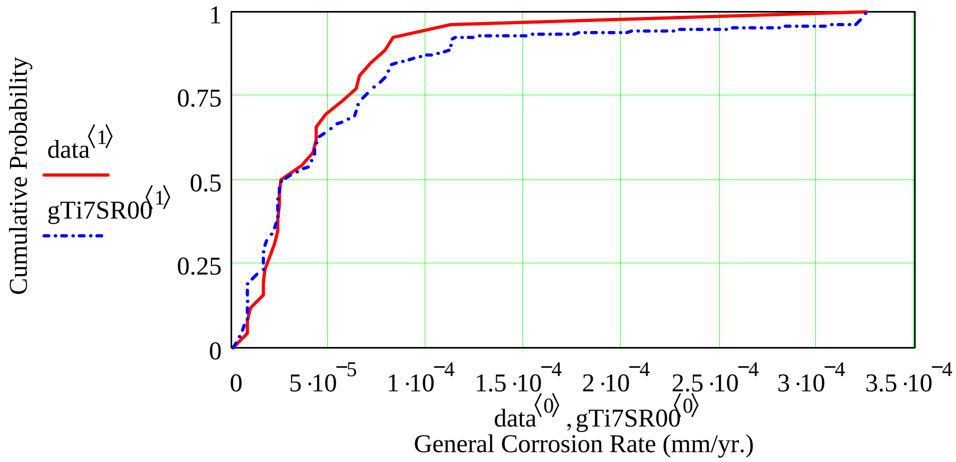
1.00000000000000E-12	0.00000000000000E+00
4.18430781465941E-06	3.84615384615385E-02
7.90540095556382E-06	7.69230769230769E-02
7.90899552966456E-06	1.15384615384615E-01
7.91733589019286E-06	1.53846153846154E-01
7.99205548612104E-06	1.92307692307692E-01
1.59679636267649E-05	2.30769230769231E-01
1.60740364754724E-05	2.69230769230769E-01
1.65389751279927E-05	3.07692307692308E-01
2.10450865748139E-05	3.46153846153846E-01
2.35658240885702E-05	3.84615384615385E-01
2.37302156627830E-05	4.23076923076923E-01
2.40329084046769E-05	4.61538461538461E-01
2.52784894494301E-05	5.00000000000000E-01
3.99976907297491E-05	5.38461538461538E-01
4.26207081441606E-05	5.76923076923077E-01
4.28647308322582E-05	6.15384615384615E-01
5.15303019184733E-05	6.53846153846154E-01
6.33683695182224E-05	6.92307692307692E-01
6.49668826549417E-05	7.30769230769231E-01
7.14961089577593E-05	7.69230769230769E-01
7.91641197726903E-05	8.07692307692307E-01
8.22028964406247E-05	8.46153846153846E-01
1.11563286061531E-04	8.84615384615384E-01
1.12788228155534E-04	9.23076923076923E-01
3.19409703501431E-04	9.61538461538461E-01
3.25000000000000E-04	1.00000000000000E+00

By changing the file names and input values to the GVP function, different cdf files are produced by the file print functions (WRITEPRN and APPENDPRN) in Mathcad.

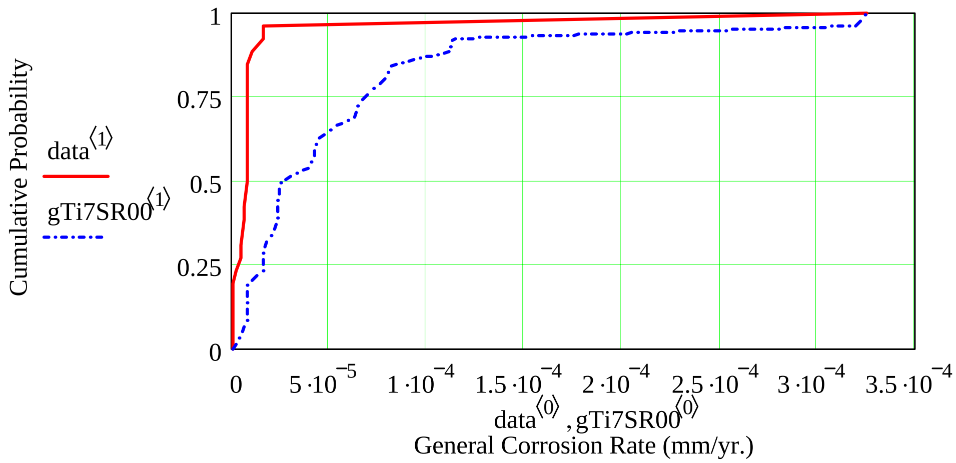
filnam := "gTiM5050.cdf "
$data := GVP\left(gTi7SR00^{\langle 1\rangle}, gTi7SR00^{\langle 0\rangle}, 0.50, 0.50, 1\right)$
WRITEPRN(filnam) := (rows(data)   cols(data))
APPENDPRN(filnam) := data



$$filnam := \text{"gTiN5050.cdf "}$$
$$data := GVP\left(gTi7SR00^{\langle 1\rangle}, gTi7SR00^{\langle 0\rangle}, 0.50, 0.50, -1\right)$$
$$WRITEPRN(filnam) := (\,rows(data) \quad cols(data)\,)$$
$$APPENDPRN(filnam) := data$$



$$filnam := \text{"gTiM7505.cdf "}$$
$$data := GVP\left(gTi7SR00^{\langle 1\rangle}, gTi7SR00^{\langle 0\rangle}, 0.75, 0.05, 1\right)$$
$$WRITEPRN(filnam) := (\,rows(data) \quad cols(data)\,)$$
$$APPENDPRN(filnam) := data$$



3.4 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

Input master file (WD4DLL.wap).

```
gTi7SR00.cdf
gTiM5050.txt
gTiN5050.txt
gTiM7505.txt
```

Input CDF for test cases (file: gTi7SR00.cdf).

```
27                        2
                  1e-012                     0
     4.1843078146594e-006    0.038461538461538
     7.9054009555638e-006    0.076923076923077
     7.9089955296646e-006     0.11538461538462
     7.9173358901929e-006     0.15384615384615
      7.992055486121e-006     0.19230769230769
     1.5967963626765e-005     0.23076923076923
     1.6074036475472e-005     0.26923076923077
     1.6538975127993e-005     0.30769230769231
     2.1045086574814e-005     0.34615384615385
      2.356582408857e-005     0.38461538461539
     2.3730215662783e-005     0.42307692307692
     2.4032908404677e-005     0.46153846153846
      2.527848944943e-005                  0.5
     3.9997690729749e-005     0.53846153846154
     4.2620708144161e-005     0.57692307692308
     4.2864730832258e-005     0.61538461538461
     5.1530301918473e-005     0.65384615384615
     6.3368369518222e-005     0.69230769230769
     6.4966882654942e-005     0.73076923076923
     7.1496108957759e-005     0.76923076923077
      7.916411977269e-005     0.80769230769231
     8.2202896440625e-005     0.84615384615385
      0.00011156328606153     0.88461538461538
      0.00011278822815553     0.92307692307692
      0.00031940970350143     0.96153846153846
                0.000325                     1
```

GVP output CDF for the first test case (file: gTiM5050.txt).

```
27
  1.0000000000E-12   0.000000000000000E+00
  7.9080728003E-06   3.846153846153800E-02
  7.9227282370E-06   7.692307692307700E-02
  8.9166513808E-06   1.153846153846200E-01
  1.5980592034E-05   1.538461538461500E-01
  1.6075475435E-05   1.923076923076900E-01
  1.6460828662E-05   2.307692307692300E-01
  1.9234298278E-05   2.692307692307700E-01
  2.1997414128E-05   3.076923076923100E-01
  2.3587950691E-05   3.461538461538500E-01
  2.3707715534E-05   3.846153846153900E-01
  2.3905721918E-05   4.230769230769200E-01
  2.4390559388E-05   4.615384615384600E-01
  2.5278489449E-05   5.000000000000000E-01
  3.4976429294E-05   5.384615384615400E-01
  4.1075553863E-05   5.769230769230800E-01
  4.2653925254E-05   6.153846153846100E-01
  4.2831705762E-05   6.538461538461500E-01
  4.7949103820E-05   6.923076923076900E-01
  5.5667093052E-05   7.307692307692299E-01
  6.3631129194E-05   7.692307692307701E-01
  6.4961801788E-05   8.076923076923100E-01
  7.0683238187E-05   8.461538461538500E-01
  7.7898693790E-05   8.846153846153800E-01
  8.1978768245E-05   9.230769230769200E-01
  1.1187640145E-04   9.615384615384600E-01
  3.2500000000E-04   1.000000000000000E+00

! Output from gvp version 1.01
! Sampled random variables U =  0.50000,qu =  0.50000
! argument in( 1) =      0.50000
! argument in( 2) =      0.50000
```

```
! argument in( 3) =      1.00000
! argument in( 4) =      1.00000
! argument in( 5) =      2.00000
```

Mathcad output CDF for the first test case (file: gTiM5050.cdf).

```
27                        2
                  1e-012                        0
     7.9080728003307e-006       0.038461538461538
     7.9227282369542e-006       0.076923076923077
     8.9166513811112e-006        0.11538461538462
     1.5980592033637e-005        0.15384615384615
     1.6075475435073e-005        0.19230769230769
     1.6460828661532e-005        0.23076923076923
     1.9234298277942e-005        0.26923076923077
      2.199741412829e-005        0.30769230769231
     2.3587950690548e-005        0.34615384615385
     2.3707715534258e-005        0.38461538461539
     2.3905721918312e-005        0.42307692307692
     2.4390559388377e-005        0.46153846153846
      2.527848944943e-005                     0.5
     3.4976429294321e-005        0.53846153846154
     4.1075553862514e-005        0.57692307692308
     4.2653925254121e-005        0.61538461538461
     4.2831705762222e-005        0.65384615384615
     4.7949103820024e-005        0.69230769230769
     5.5667093052459e-005        0.73076923076923
     6.3631129193739e-005        0.76923076923077
     6.4961801788385e-005        0.80769230769231
     7.0683238186706e-005        0.84615384615385
     7.7898693789344e-005        0.88461538461538
       8.19787682444e-005        0.92307692307692
      0.00011187640144994        0.96153846153846
                0.000325                        1
```

GVP output CDF for the second test case (file: gTiN5050.txt).

```
27
  1.0000000000E-12   0.000000000000000E+00
  7.9080729562E-06   3.846153846153800E-02
  7.9227517980E-06   7.692307692307700E-02
  9.2535733347E-06   1.153846153846200E-01
  1.5980628924E-05   1.538461538461500E-01
  1.6075496082E-05   1.923076923076900E-01
  1.6461749708E-05   2.307692307692300E-01
  1.9362461435E-05   2.692307692307700E-01
  2.2031225218E-05   3.076923076923100E-01
  2.3588017360E-05   3.461538461538500E-01
  2.3707782923E-05   3.846153846153900E-01
  2.3906188955E-05   4.230769230769200E-01
  2.4397046701E-05   4.615384615384600E-01
  2.5278489449E-05   5.000000000000000E-01
  3.5694618764E-05   5.384615384615400E-01
  4.1095792129E-05   5.769230769230800E-01
  4.2654007281E-05   6.153846153846100E-01
  4.2831787163E-05   6.538461538461500E-01
  4.8140240689E-05   6.923076923076900E-01
  5.5950749656E-05   7.307692307692299E-01
  6.3633879490E-05   7.692307692307701E-01
  6.4961864359E-05   8.076923076923100E-01
  7.0716507075E-05   8.461538461538500E-01
  7.7951300826E-05   8.846153846153800E-01
  8.1982636492E-05   9.230769230769200E-01
  1.1187767631E-04   9.615384615384600E-01
  3.2500000000E-04   1.000000000000000E+00

! Output from gvp version 1.01
```

```
! Sampled random variables U =  0.50000,qu =  0.50000
! argument in( 1) =      0.50000
! argument in( 2) =      0.50000
! argument in( 3) =     -1.00000
! argument in( 4) =      1.00000
! argument in( 5) =      3.00000
```

Mathcad output CDF for the second test case (file: gTiN5050.cdf).

```
27                       2
                 1e-012                       0
     7.9080729562145e-006      0.038461538461538
     7.9227517980398e-006      0.076923076923077
     9.2535733350887e-006       0.11538461538462
      1.598062892411e-005       0.15384615384615
     1.6075496081667e-005       0.19230769230769
     1.6461749707824e-005       0.23076923076923
     1.9362461435011e-005       0.26923076923077
     2.2031225218071e-005       0.30769230769231
     2.3588017359715e-005       0.34615384615385
     2.3707782922977e-005       0.38461538461539
      2.390618895497e-005       0.42307692307692
     2.4397046700807e-005       0.46153846153846
      2.527848944943e-005                    0.5
     3.5694618764105e-005       0.53846153846154
     4.1095792128698e-005       0.57692307692308
     4.2654007280659e-005       0.61538461538461
     4.2831787162801e-005       0.65384615384615
     4.8140240689419e-005       0.69230769230769
     5.5950749655974e-005       0.73076923076923
     6.3633879490256e-005       0.76923076923077
     6.4961864359164e-005       0.80769230769231
     7.0716507075003e-005       0.84615384615385
     7.7951300826115e-005       0.88461538461538
     8.1982636491457e-005       0.92307692307692
      0.00011187767631254       0.96153846153846
                 0.000325                      1
```

GVP output CDF for the third test case (file: gTiM7505.txt).

```
27
  1.0000000000E-12   0.000000000000000E+00
  6.3582282761E-11   3.846153846153800E-02
  6.3446588157E-10   7.692307692307700E-02
  5.0326740107E-09   1.153846153846200E-01
  3.6855544470E-08   1.538461538461500E-01
  2.6487663977E-07   1.923076923076900E-01
  1.9342192774E-06   2.307692307692300E-01
  4.4095920679E-06   2.692307692307700E-01
  4.8110822300E-06   3.076923076923100E-01
  5.2662267575E-06   3.461538461538500E-01
  5.7875359227E-06   3.846153846153900E-01
  6.3910264402E-06   4.230769230769200E-01
  7.0976697807E-06   4.615384615384600E-01
  7.9054224445E-06   5.000000000000000E-01
  7.9060976482E-06   5.384615384615400E-01
  7.9068263259E-06   5.769230769230800E-01
  7.9076192799E-06   6.153846153846100E-01
  7.9084905343E-06   6.538461538461500E-01
  7.9100698220E-06   6.923076923076900E-01
  7.9126008365E-06   7.307692307692299E-01
  7.9155056342E-06   7.692307692307701E-01
  7.9314566958E-06   8.076923076923100E-01
  7.9685378684E-06   8.461538461538500E-01
  9.9711015058E-06   8.846153846153800E-01
  1.5988963043E-05   9.230769230769200E-01
  1.6378897834E-05   9.615384615384600E-01
```

```
  3.2500000000E-04   1.000000000000000E+00

! Output from gvp version 1.01
! Sampled random variables U =  0.75000,qu =  0.05000
! argument in( 1) =      0.75000
! argument in( 2) =      0.05000
! argument in( 3) =      1.00000
! argument in( 4) =      1.00000
! argument in( 5) =      4.00000
```

Mathcad output CDF for the third test case (file: gTiM7505.cdf).

```
27                        2
                  1e-012                        0
      6.358228274309e-011       0.038461538461538
     6.3446588136749e-010       0.076923076923077
     5.0326740085247e-009        0.11538461538462
     3.6855544450271e-008        0.15384615384615
     2.6487663952877e-007        0.19230769230769
     1.9342192756676e-006        0.23076923076923
     4.4095920677552e-006        0.26923076923077
     4.8110822298146e-006        0.30769230769231
     5.2662267572752e-006        0.34615384615385
     5.7875359224077e-006        0.38461538461539
     6.3910264399033e-006        0.42307692307692
     7.0976697803494e-006        0.46153846153846
     7.9054224445177e-006                     0.5
     7.9060976482158e-006        0.53846153846154
     7.9068263258645e-006        0.57692307692308
     7.9076192798641e-006        0.61538461538461
     7.9084905342771e-006        0.65384615384615
     7.9100698220167e-006        0.69230769230769
     7.9126008365061e-006        0.73076923076923
     7.9155056341654e-006        0.76923076923077
     7.9314566957708e-006        0.80769230769231
     7.9685378683526e-006        0.84615384615385
     9.9711015042821e-006        0.88461538461538
     1.5988963043273e-005        0.92307692307692
     1.6378897834273e-005        0.96153846153846
                0.000325                        1
```

4. REFERENCES

CRWMS M&O 1999f. *Testing of Software Routine to Determine Deviate and Cumulative Probability: ModStandardNormal Version 1.0.* CAL-EBS-MD-000004 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991018.0213.

Deutsch, C.V. and Journel, A.G. 1992. *GSLIB Geostatistical Software Library and User's Guide.* New York, New York: Oxford University Press. TIC: 224174.

Golder Associates 2000. *User's Guide, GoldSim, Graphical Simulation Environment.* Version 6.02. Manual Draft #4 (March 17, 2000). Redmond, Washington: Systems Simulation Group Golder Associates Inc. TIC: 247347.

ATTACHMENT II

MFD SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Name and Version Number - MFD (ManuFacturing Defects), version 1.01

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 5.0, Standard Edition.

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

2. DESCRIPTION AND TESTING

The software routine MFD calculates the cumulative probability distribution for the occurrence and size of manufacturing defects in the closure weld of waste packages given the non-detection probability and the fraction of surface breaking flaws. These calculations are based on the abstraction of flaw density and size distribution discussed in the Manufacturing Defects Calculation (CRWMS M&O 2000g). The outputs of MFD are:

- A text file containing the cumulative distribution function (CDF) table for the number cracks (given that one or more cracks have occurred),
- A text file containing the CDF table for crack sizes, and
- An output argument containing the probability of at least one crack occurring.

2.1 DESCRIPTION OF SOFTWARE ROUTINE AND THE EXECUTION ENVIRONMENT

The MFD source code is a Fortran program 373 lines in length. It conforms to the Fortran 90 standard and is thus highly portable. MFD was developed and tested in the Windows NT 4.0 operating system, and has been compiled with Visual Fortran 5.0, Standard Edition for Microsoft Windows 32 bit operating system environments. MFD may compile as a dynamic link library (MFD.DLL), which may be coupled with computer codes through external element mechanisms. MFD directly links and runs to simulate randomly occurring manufacturing defects for modeling waste package failures. The outputs are used by other Total System Performance codes to generate distributions for waste package failures.

The CDF file formats consists of a first line containing the number of rows in the CDF lookup table with the following lines containing two columns of numbers. The first column of numbers is the distribution values in increasing order. The second column contains the cumulative probability values.

Compilation of MFD requires several Fortran modules to be present from the WAPDEG library (CRWMS M&O 1999f). These are modDefaultSize and modStandardNormal.

The bulk of MFD's coding is devoted to computing the cumulative probability of a manufacturing defect conditional to (based on) the probability for the non-detection of weld flaws. The parameters *b* and • define the probability for non-detection. This calculation also requires ψ the fraction of surface breaking fractures (Section 5). The inputs are read as part of the argument list of MFD, as the elements of array in(*):

in(1) = closure lid (weld) thickness (mm)
in(2) = closure lid radius (m)
in(3) = *b*, the location parameter of the non-detection probability
in(4) = • , the scale parameter of the non-detection probability
in(5) = ψ, the fraction of surface breaking fractures
in(6) = file index for the output file for CDF for the number of cracks
in(7) = file index for the output file for CDF for the size of cracks

The last two inputs are indices (line numbers) within a reference list file (WD4DLL.WAP) for filenames used by several DLLs (MFD being one) for waste package simulation.

The output consists of the CDFs written to the files indexed in(6) and in(7), and the probability of at least one crack per waste package (written to out(1)). The MFD DLL follows a project-coding standard that requires all DLL's to accept as input a method variable that controls the operation of the program. If a DLL is called with the following values of method, the following will occur:

method = 0	Initialize (MFD requires no initialization, thus nothing happens).
method = 1	Normal calculation (for MFD, compute the CDFs and probability of at least one crack occurring).
method = 2	Report the version number as out(1).
method = 3	Report the number of input and output arguments as out(1) and out(2), respectively (for MFD, this should yield the values 7 and 1, respectively).
method = 99	Clean up, close any open files.

2.2 DESCRIPTION OF THE ALGORITHM

MFD receives the input parameters from the argument list, and then follows the algorithm presented in the Manufacturing Defects Calculation (CRWMS M&O 2000g). Specifically, the following steps are performed:

1. Compute the conditional probability that the flaw is not detected, $\Pr(B \mid b, v)$. This is done numerically, via Rhomberg integration (Press et al. 1992).
2. Calculate $\lambda(\psi, b, v)$, the Poisson parameter rate for the number of cracks per closure weld.
3. Calculate the probability of at least one or more cracks per closure weld, pass this to out(1).
4. Evaluate the conditional (given one or more cracks have occurred) CDF for the number of cracks as a Poisson process with parameter $\lambda(\psi, b, v)$. Write the result to the file specified through in(6).
5. Evaluate the CDF of crack sizes, $G(s \mid b, v)$, as the convolution of the probability of non-detection (PND) and the flaw size distribution, divided by $\Pr(B \mid b, v)$. This is done

numerically, via Rhomberg integration (Press et al. 1992). Write the result to the file specified through in(7).

2.3 DESCRIPTION OF TEST CASE

The testing approach involves comparing the results of executing MFD and comparing the results with the example calculations presented in Attachment II of the Manufacturing Defects Calculation (CRWMS M&O 2000g). The specific test case is to calculate the CDFs and the probability of at least one crack, given $P_{ND}(5,3)$ and ψ = 0.0034. The output CDFs and probability should be a reasonable match to the numerical results for this case in Attachment II of the Manufacturing Defects Calculation (CRWMS M&O 2000g).

Running the MFD as a DLL, the following values are inserted as data elements in the MFD input stream:

in(1) = 10	thck
in(2) = 0.76	r
in(3) = 5	b
in(4) = 3	v
in(5) = 0.0034	ψ
in(6) = 3	idxnum
in(7) = 4	idxsiz

The test case requires one input file, a text file WD4DLL.wap, which is a list of filenames to be read by MFD. A listing of WD4DLL.wap is provided in Section 3. The third and fourth lines are the names of files used by MFD for the output CDFs for the number of cracks and the size of cracks, respectively.

2.4 DESCRIPTION OF TEST RESULTS

Comparison of the test case output files with those in Attachment II of the Manufacturing Defects Calculation (CRWMS M&O 2000g) confirm that the MFD gives the anticipated results. The results also indicate that the probability of at least one crack should be 0.13718317. The output CDFs and probability are in agreement.

2.5 RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED

The preceding test case evaluates MFD for a typical set of parameters as observed from the manufacturing data

The waste package lid / weld thickness, for 10 and 25 (mm).
The waste package lid radius, for 0.76 (m).
The location parameter of the non-detection probability, *b*: for values 1.6 to 5 (mm).
The shape parameter of the non-detection probability, • for values 1 to 3.
The fraction of surface breaking fractures, ψ for values 0.0013 to 0.0049.

2.6 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

MFD will execute properly if the following ranges and types of parameter values are met:

The waste package lid / weld thickness, a real number in the range 6.35 to 12.7 (mm) or the range 19.05 to 25.4 (mm). Other thickness ranges are not supported at this time.
The waste package lid radius, a positive real number in meters.
The location parameter of the non-detection probability, *b*: a positive real number (mm)
The shape parameter of the non-detection probability, • : a positive real number
The fraction of surface breaking fractures, ψ: a positive real number in the range 0 to 1.0

3. SUPPORTING INFORMATION

3.1 DIRECTORY LISTING OF EXECUTABLES AND DATA FILES

```
03/16/00  12:49p  mfd.f
03/16/00  11:35a  mfd.dll
03/16/00  03:05p  mfdcall.f
03/16/00  03:05p  mfdcall.exe
03/16/00  03:07p  mfdcall.out
01/27/00  01:54p  WD4DLL.wap
03/16/00  03:07p  WDMFD1test.txt
03/16/00  03:07p  WDMFD2test.txt
```

3.2 COMPUTER LISTING OF SOURCE CODE

```
SUBROUTINE mfd(method, state, in, out)
!
!  Subroutine to calculate the cdfs for canister defect occurrence
!  and size. This subroutine performs the following functions:
!  1. Argument list:
!      thck   closure lid (weld) thickness
!      r      closure lid radius
!      b      Location parameter for PND (probability of
!             nondetection) function (Uniform random variable)
!      v      Shape parameter for PND distribution
!             (Uniform random variable)
!      psi    Fraction of Surface Breaking Flaws.
!             (Uniform random variable)
!      idxnum File index for output conditional CDF
!             of number of cracks per WP.
!      idxsiz File index for output CDF of crack sizes
!  2. Calculate/Output:
!      CDF of number of cracks per WP (to file: numcdf).
!      CDF of crack sizes (to file: sizcdf).
!      flaw probability of one or more cracks per WP (to out(1)).
!
!DEC$ ATTRIBUTES dllexport,c :: mfd
!DEC$ ATTRIBUTES ALIAS : "mfd" :: mfd
!DEC$ ATTRIBUTES value       :: method
!DEC$ ATTRIBUTES reference   :: state
!DEC$ ATTRIBUTES reference   :: in
!DEC$ ATTRIBUTES reference   :: out
```

```
      USE ModDefaultsize
      USE ModStandardNormal
      IMPLICIT NONE
      integer(IKind) :: method   ! input, tells mfd what to do
      integer(IKind) :: state    ! return, 0 = OK
      real(RKind)    :: in(*)    ! input arguments
      real(RKind)    :: out(*)   ! output arguments
      real(RKind), PARAMETER :: VERSION = 1.01
      integer(IKind), PARAMETER :: NUMIN = 7, NUMOUT = 1
      integer(IKind), PARAMETER :: NSIZE = 200
      real(RKind), PARAMETER :: PI = 3.141592653589793
      integer(IKind) :: outunit, errunit, idxnum, idxsiz
      character(LEN = 80) :: numcdf, sizcdf, line1
      integer(IKind) :: n, i
      real(RKind) :: thck, r, b, v, psi, PrBbv, Lpbv, PrSbv, GSbv
      real(RKind) :: up, eps0, p0, p, size, step1, med, sdev, rdctn
      real(RKind) :: cpr(NSIZE)
!
!**********************************************************************
!
      if (method .eq. 0) then        ! Initialize
        state = 0
        return
      elseif (method .eq. 2) then    ! Report code version
        out(1) = VERSION
        state = 0
        return
      elseif (method .eq. 3) then    ! Report number of arguments
        out(1) = NUMIN
        out(2) = NUMOUT
        state = 0
        return
      elseif (method .eq. 1) then    ! Calculate
        thck   = in(1)
        r      = in(2)
        b      = in(3)
        v      = in(4)
        psi    = in(5)
        idxnum = in(6)
        idxsiz = in(7)
!
!  Open the file list and find the I/O filenames
!
        outunit = nextfreeunit()
        open(unit = outunit, file = 'WD4DLL.WAP')
        n = max(idxnum, idxsiz)
        do i = 1, n
          read(outunit,*) line1
          if (i .eq. idxnum) numcdf  = line1
          if (i .eq. idxsiz) sizcdf  = line1
        end do
        close(unit = outunit)
!
!  Evaluate the conditional probability Pr(B|b,v)
!  up   = upper bound of integration
!  eps0 = lower bound of integration
!  LOOK OUT HERE, ADJUSTING BOUNDS
```

```
!
        up = 8.0
        eps0 = 1.0E-20
        med = 0.1159*25.4 + thck*(-0.0445 + thck*0.00797/25.4)
        sdev = 0.09733 + thck*(0.3425 - thck*0.07288/25.4)/25.4
        call qromb(eps0, up, b, v, med, sdev, PrBbv, state)
        if (state .eq. 1_IKind) then
          errunit = nextfreeunit()
          open(unit = errunit, file = 'mfderror.log')
          write(errunit,*) 'Failure of qromb, 93'
          close(unit = errunit)
          return
        end if
!
!  Calculate the Poisson parameter (Lpbv)
!
        if ((thck .ge. 19.05) .and. (thck .le.25.4)) then
          rdctn = (60*thck - 635)/889
        else if  ((thck .ge. 6.35) .and. (thck .le. 12.7)) then
          rdctn = (-218*thck + 5207)/2845
        else
          errunit = nextfreeunit()
          open(unit = errunit, file = 'mfderror.log')
          write(errunit,*) 'Thickness out of range, method = ',method
          close(unit = errunit)
          state = 1
          return
        end if
        Lpbv = 0.6839*(12.8 + 31.4*psi)*rdctn*(2*PI*r)*psi*PrBbv
!
!  Evaluate the cumulative conditional probability distribution
!  of crack occurrence as a cumulative Poisson distribution and
!  write to file (numcdf).
!
        p0 = exp(-1.0_RKind*Lpbv)
        out(1) = 1.0_RKind - p0
        n = 1
        p = p0*Lpbv
        cpr(1) = p
        do while ((p .gt. 1.0D-14) .and. (n .lt. NSIZE))
          n = n+1
          p = p*Lpbv/dble(n)
          cpr(n) = cpr(n-1) + p
        end do
        outunit = nextfreeunit()
        open(unit = outunit, file = numcdf)
        write(outunit,*) 2*n
        write(outunit,'(1x,I11,1x,f18.15)') 1, 0.0
        do i = 1, n-1
          write(outunit,*) i, cpr(i)/out(1)
          write(outunit,*) i+1, cpr(i)/out(1)
        end do
        write(outunit,*) n, cpr(n)/out(1)
        write(outunit,*)
        write(outunit,3330) VERSION
        write(outunit,3331) out(1)
        write(outunit,3338) ( i, in(i), i = 1, NUMIN )
```

```
        write(outunit,*)
 3330   format('! Output from mfd version ',F4.2)
 3331   format('! For probability of flaw =',F12.8)
 3338   format('! argument in(',I2,') = ',f12.5)
        close(unit = outunit)
!
!  Evalulate the cumulative probability distribution of
!  crack sizes, G(s|b,v) and write to file (sizcdf).
!
        size = 0.0
        step1 = up/NSIZE
        outunit = nextfreeunit()
        open(outunit, file = sizcdf)
        write(outunit,*) NSIZE
        do i = 1, NSIZE
          size = size + step1
          call qromb (eps0, size, b, v, med, sdev, PrSbv, state)
          if (state .eq. 1_IKind) then
            errunit = nextfreeunit()
            open(unit = errunit, file = 'mfderror.log')
            write(errunit,*) 'Failure of qromb, 155'
            close(errunit)
            close(outunit)
            return
          end if
          GSbv = PrSbv / PrBbv
          write(outunit,*) size, GSbv
        end do
        write(outunit,*)
        write(outunit,3330) VERSION
        write(outunit,3331) out(1)
        write(outunit,3338) ( i, in(i), i = 1, NUMIN )
        write(outunit,*)
        close(unit = outunit)
        state = 0
        return
      elseif (method .eq. 99) then   ! Shut-down
        close(unit = outunit)
        close(unit = errunit)
        state = 0
        return
      else
        errunit = nextfreeunit()
        open(unit = errunit, file = 'mfderror.log')
        write(errunit,*) 'mfd crashed, method = ',method
        close(unit = errunit)
        state = 1
        return
      end if                         ! end block for method
      CONTAINS     ! qromb, polint, trapzd, nextfreeunit
!
!**********************************************************************
!
      SUBROUTINE qromb(a, b, p1, p2, p3, p4, ss, state)
!
!  Numerical integration of function 'pndf' from a to b via
!  Rhomberg integration, as described in Numerical Recipes Section 4.3.
```

```
!  Calls: polint, trapzd
!
      USE ModDefaultsize
      real(RKind) :: a, b, p1, p2, p3, p4, ss
      integer(IKind) :: state
      integer(IKind), PARAMETER :: JMAX = 30, JMAXP = JMAX+1
      integer(IKind), PARAMETER :: K = 5, KM = K-1
      real(RKind), PARAMETER :: EPS = 1.0e-12
      integer(IKind) :: j
      real(RKind) :: dss, h(JMAXP), s(JMAXP)

      h(1) = 1.0
      do j = 1, JMAX
        call trapzd(a,b,p1,p2,p3,p4,s(j),j)
        if (j .ge. K) then
          call polint(h(j-KM),s(j-KM),K,0,ss,dss,state)
          if (state .eq. 1_IKind) return
          if (abs(dss) .le. EPS*abs(ss)) return
        endif
        s(j+1) = s(j)
        h(j+1) = 0.25*h(j)
      end do
      state = 1   ! too many steps in qromb.
      return
      END SUBROUTINE qromb
!
!**********************************************************************
!
      SUBROUTINE polint(xa, ya, n, x, y, dy, state)
!
!  Polynomial interpolation for y given arrays xa and ya
!  (each of size n).  See Numerical Recipes Section 3.1
!  Calls: None
!
      USE ModDefaultsize
      integer(IKind), PARAMETER :: NMAX = 10
      integer(IKind) :: n, x, state
      real(RKind) :: dy, y, xa(n), ya(n)
      integer(IKind) :: i, m, ns
      real(RKind) :: den, dif, dift, ho, hp, w, c(NMAX), d(NMAX)
c
      ns = 1
      dif = abs(x-xa(1))
      do i = 1, n
        dift = abs(x-xa(i))
        if (dift .lt. dif) then
          ns = i
          dif = dift
        endif
        c(i) = ya(i)
        d(i) = ya(i)
      end do
      y = ya(ns)
      ns = ns-1
      do m = 1, n-1
        do i = 1, n-m
          ho = xa(i)-x
```

```
          hp = xa(i+m)-x
          w = c(i+1)-d(i)
          den = ho-hp
          if (den .eq. 0.) then
            state = 1  ! failure in polint.
            return
          end if
          den = w/den
          d(i) = hp*den
          c(i) = ho*den
        end do
        if (2*ns .lt. n-m) then
          dy = c(ns+1)
        else
          dy = d(ns)
          ns = ns-1
        endif
        y = y+dy
      end do
      return
      END SUBROUTINE polint
!
!**********************************************************************
!
      SUBROUTINE trapzd(a,b,p1,p2,p3,p4,s,n)
!
!  Evaluates trapezoidal rule for function pndf from a to b.
!  See Numerical Recipes Section 4.2.
!  Calls:
!  pndf(indep.variable, parameter1, parameter2, parameter3, parameter4)
!
      USE ModDefaultsize
      integer(IKind) :: n
      real(RKind) :: a, b, p1, p2, p3, p4, s
      integer(IKind) :: it, j
      real(RKind) :: del, sum, tnm, x
!
      if (n .eq. 1) then
        s = 0.5*(b-a)*(pndf(a,p1,p2,p3,p4)+pndf(b,p1,p2,p3,p4))
      else
        it = 2**(n-2)
        tnm = it
        del = (b-a)/tnm
        x = a + 0.5*del
        sum = 0.
        do j = 1, it
          sum = sum + pndf(x,p1,p2,p3,p4)
          x = x + del
        end do
        s = 0.5*( s + (b-a)*sum/tnm )
      endif
      return
      END SUBROUTINE trapzd
!
!**********************************************************************
!
      real(RKind) FUNCTION pndf(s,b,v,med,sdev)
```

```
!
!  Calculates the integrand PND(s).f(s) used in the
!  integral for the conditional probability Pr(B|b,v).
!  Uses Erf(), the error function, from ModStandardNormal.
!
!  Input:  s     crack size (mm)
!          b     location parameter of PND
!          v     shape parameter of PND
!          med   location parameter of f
!          sdev  shape parameter of f
!  Output: (function value)
!
      real(RKind), PARAMETER :: P=0.005, PI=3.141592653589793
      real(RKind) :: s, b, v, med, sdev
      real(RKind) :: pnd, f
!
      if (s .le. 0) then
        stop !crack length invalid
        return
      end if
!
!  Calculate PND(s) and f(s)
!
      pnd = ( (P+1.0)/2.0 + (P-1.0)*Erf(.true.,v*log(s/b) )/2.0)
     +    * ( (P+1.0)/2.0 + (P-1.0)*Erf(.true.,v*log(s/b) )/2.0)
      f = (log(s/med))*(log(s/med)) / (2.0*sdev*sdev)
      f = exp(-f) / (s*sdev*sqrt(2*PI))
      pndf = pnd*f
      return
      END FUNCTION pndf
!
!**********************************************************************
!
      integer(IKind) FUNCTION nextfreeunit()
!
!  Find the smallest unit number not currently attached and in use.
!  Avoid units 5 and 6.
!  Input : (none)
!  Output: (function value)
!  Local : i, InUse
!
!  Local variables
!
      integer(IKind) :: i
      logical InUse
!
      InUse = .true.
      i = 0
      do while (InUse)
        i = i + 1
        if(i .ne. 5 .and. i .ne. 6) then
          inquire(i, opened = InUse)
        end if
      end do
      nextfreeunit = i
      RETURN
      END FUNCTION nextfreeunit
```

```
!
!*********************************************************************
!
      END SUBROUTINE mfd
```

3.3 COMPUTER LISTING OF SOURCE CODE FOR TEST CALLER

Text of file mfdcall.f

```
PROGRAM mfdcall
!
!  Driver to test DLL mfd
!
      IMPLICIT NONE
      integer, PARAMETER :: intkind=4, rlkind=8
      integer(intkind), PARAMETER :: MAXIN = 7, MAXOUT = 2
      integer(intkind)  :: state       ! return, 0 = OK
      real(rlkind)      :: in(MAXIN)   ! input arguments
      real(rlkind)      :: out(MAXOUT) ! output arguments
!
      INTERFACE
        SUBROUTINE mfd(method, state, in, out)
        !DEC$ ATTRIBUTES DLLIMPORT :: mfd
        !DEC$ ATTRIBUTES ALIAS : "mfd" :: mfd
        !DEC$ ATTRIBUTES value :: method
        !DEC$ ATTRIBUTES reference :: state
        !DEC$ ATTRIBUTES reference :: in
        !DEC$ ATTRIBUTES reference :: out
        integer, PARAMETER :: intkind = 4, rlkind = 8
        integer(intkind)  :: method
        integer(intkind)  :: state   ! return, 0 = OK
        real(rlkind)      :: in(*)   ! input arguments
        real(rlkind)      :: out(*)  ! output arguments
        END SUBROUTINE mfd
      END INTERFACE
!
!  Initialize and
!  Assign test values to in array
!
      open(12,file='mfdcall.out')
      state = 0
      in(1) = 10        ! thck
      in(2) = 0.76      ! r
      in(3) = 5         ! b
      in(4) = 3         ! v
      in(5) = 0.0034    ! fraction of flaws
      in(6) = 3         ! idxnum
      in(7) = 4         ! idxsiz
!
!  Call DLL with calling sequence for method = 2, 3, 0, 1, 99
!
      CALL mfd(2, state, in, out)
      write(12,*) 'method = 2 run'
      write(12,121) out(1)
 121  format(1x,'version number:',f5.2)

      CALL mfd(3, state, in, out)
```

```
      write(12,*) 'method = 3 run'
      write(12,122) out(1), out(2)
 122  format(1x,'number of input and output arguments:',2f5.1)

      CALL mfd(0, state, in, out)
      write(12,*) 'method = 0 run'

      CALL mfd(1, state, in, out)
      write(12,*) 'method = 1 run'
      write(12,*) 'probability of at least one crack occurring =',out(1)

      CALL mfd(99,state, in, out)
      write(12,*) 'method = 99 run'

      END PROGRAM mfdcall
```

3.4 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

Input text file (WD4DLL.wap).

```
WDMFD1gsim.txt
WDMFD2gsim.txt
WDMFD1test.txt
WDMFD2test.txt
```

Output text file of caller (mfdcall.out).

```
method = 2 run
version number: 1.01
method = 3 run
number of input and output arguments:  7.0  1.0
method = 0 run
method = 1 run
probability of at least one crack occurring =  0.137183171223015
method = 99 run
```

Output CDF for the number of cracks (file: WDMFD1test.txt).

```
20
           1  0.000000000000000
           1  0.928037232675321
           2  0.928037232675321
           2  0.996504506467805
           3  0.996504506467805
           3  0.999872020482346
           4  0.999872020482346
           4  0.999996242063074
           5  0.999996242063074
           5  0.999999907912968
           6  0.999999907912968
           6  0.999999998064074
           7  0.999999998064074
           7  0.999999999964367
           8  0.999999999964367
           8  0.999999999999416
```

```
           9  0.999999999999416
           9  0.999999999999991
          10  0.999999999999991
          10   1.00000000000000

! Output from mfd version 1.01
! For probability of flaw =  0.13718317
! argument in( 1) =     10.00000
! argument in( 2) =      0.76000
! argument in( 3) =      5.00000
! argument in( 4) =      3.00000
! argument in( 5) =      0.00340
! argument in( 6) =      3.00000
! argument in( 7) =      4.00000
```

Output CDF for the crack size (file: WDMFD2test.txt).

```
         200
  4.000000000000000E-002  6.122514873113449E-079
  8.000000000000000E-002  2.075328338612312E-055
  0.120000000000000       1.277161357176911E-043
  0.160000000000000       3.869600351908593E-036
  0.200000000000000       7.699163815038370E-031
  0.240000000000000       7.747981450177105E-027
  0.280000000000000       1.107948715129825E-023
  0.320000000000000       4.059079696319943E-021
  0.360000000000000       5.490443441651299E-019
  0.400000000000000       3.488297111033730E-017
  0.440000000000000       1.229208276756130E-015
  0.480000000000000       2.706166806296714E-014
  0.520000000000000       4.064257809297995E-013
  0.560000000000000       4.450509757610495E-012
  0.600000000000000       3.741005359287602E-011
  0.640000000000000       2.513685027270116E-010
  0.680000000000000       1.394589155763339E-009
  0.720000000000000       6.558422864012984E-009
  0.760000000000000       2.671328726614129E-008
  0.800000000000000       9.593776334480947E-008
  0.840000000000000       3.083775706138229E-007
  0.880000000000000       8.984484440126560E-007
  0.920000000000000       2.398225321282131E-006
  0.960000000000000       5.919369519086295E-006
   1.00000000000000       1.361765368024870E-005
   1.04000000000000       2.940132588232341E-005
   1.08000000000000       5.993548921316788E-005
   1.12000000000000       1.159703286694620E-004
   1.16000000000000       2.139814228382318E-004
   1.20000000000000       3.780592782246839E-004
   1.24000000000000       6.419297335403709E-004
   1.28000000000000       1.050936195250956E-003
   1.32000000000000       1.663778182569343E-003
   1.36000000000000       2.553786020741825E-003
   1.40000000000000       3.809523058259494E-003
   1.44000000000000       5.534544714393358E-003
   1.48000000000000       7.846204143358305E-003
   1.52000000000000       1.087347023069049E-002
   1.56000000000000       1.475380597286370E-002
   1.60000000000000       1.962923454571276E-002
   1.64000000000000       2.564178800143392E-002
   1.68000000000000       3.292858301915785E-002
   1.72000000000000       4.161679557060067E-002
   1.76000000000000       5.181881063633921E-002
   1.80000000000000       6.362780565138877E-002
   1.84000000000000       7.711399062200439E-002
   1.88000000000000       9.232167862766107E-002
```

1.92000000000000	0.109267303114631
1.96000000000000	0.127938438383570
2.00000000000000	0.148293821806663
2.04000000000000	0.170264324503798
2.08000000000000	0.193754774282099
2.12000000000000	0.218646502270619
2.16000000000000	0.244800463458531
2.20000000000000	0.272060770950807
2.24000000000000	0.300258483157525
2.28000000000000	0.329215490810680
2.32000000000000	0.358748364858505
2.36000000000000	0.388672045039880
2.40000000000000	0.418803270474302
2.44000000000000	0.448963676280657
2.48000000000000	0.478982502678221
2.52000000000000	0.508698884133359
2.56000000000000	0.537963705101794
2.60000000000000	0.566641025266618
2.64000000000000	0.594609090626320
2.68000000000000	0.621760957293407
2.72000000000000	0.648004762536794
2.76000000000000	0.673263682673004
2.80000000000000	0.697475620193743
2.84000000000000	0.720592663363894
2.88000000000000	0.742580360799379
2.92000000000000	0.763416851593951
2.96000000000000	0.783091888734866
3.00000000000000	0.801605790119737
3.04000000000000	0.818968347714560
3.08000000000000	0.835197721454892
3.12000000000000	0.850319340599759
3.16000000000000	0.864364831454154
3.20000000000000	0.877370986827128
3.24000000000000	0.889378789310906
3.28000000000000	0.900432497498173
3.32000000000000	0.910578801611457
3.36000000000000	0.919866052701278
3.40000000000000	0.928343567568646
3.44000000000000	0.936061009865649
3.48000000000000	0.943067846405322
3.52000000000000	0.949412876544520
3.56000000000000	0.955143831568140
3.60000000000000	0.960307040275434
3.64000000000000	0.964947156426161
3.68000000000000	0.969106943324583
3.72000000000000	0.972827110581832
3.76000000000000	0.976146197982662
3.80000000000000	0.979100501373868
3.84000000000000	0.981724035571688
3.88000000000000	0.984048529439053
3.92000000000000	0.986103448497482
3.96000000000000	0.987916040698552
4.00000000000000	0.989511401275907
4.04000000000000	0.990912552919336
4.08000000000000	0.992140537848057
4.12000000000000	0.993214518703309
4.16000000000000	0.994151885522761
4.20000000000000	0.994968366394957
4.24000000000000	0.995678139716321
4.28000000000000	0.996293946281525
4.32000000000000	0.996827199726896
4.36000000000000	0.997288094114340
4.40000000000000	0.997685707687733
4.44000000000000	0.998028102054014
4.48000000000000	0.998322416238020
4.52000000000000	0.998574955232143
4.56000000000000	0.998791272811616
4.60000000000000	0.998976248513566
4.64000000000000	0.999134158784609
4.68000000000000	0.999268742389693
4.72000000000000	0.999383260245342

4.76000000000000	0.999480549895161
4.80000000000000	0.999563074886746
4.84000000000000	0.999632969338268
4.88000000000000	0.999692078001529
4.92000000000000	0.999741992138546
4.96000000000000	0.999784081531383
5.00000000000000	0.999819522941533
5.04000000000000	0.999849325327599
5.08000000000000	0.999874352118048
5.12000000000000	0.999895340821726
5.16000000000000	0.999912920242653
5.20000000000000	0.999927625547960
5.24000000000000	0.999939911419977
5.28000000000000	0.999950163505180
5.32000000000000	0.999958708354524
5.36000000000000	0.999965822032257
5.40000000000000	0.999971737553482
5.44000000000000	0.999976651294521
5.48000000000000	0.999980728505515
5.52000000000000	0.999984108040347
5.56000000000000	0.999986906406371
5.60000000000000	0.999989221224604
5.64000000000000	0.999991134180148
5.68000000000000	0.999992713533065
5.72000000000000	0.999994016251172
5.76000000000000	0.999995089818271
5.80000000000000	0.999995973764492
5.84000000000000	0.999996700959277
5.88000000000000	0.999997298701854
5.92000000000000	0.999997789639476
5.96000000000000	0.999998192539461
6.00000000000000	0.999998522937159
6.04000000000000	0.999998793677942
6.08000000000000	0.999999015376093
6.12000000000000	0.999999196788782
6.16000000000000	0.999999345136716
6.20000000000000	0.999999466367622
6.24000000000000	0.999999565376239
6.28000000000000	0.999999646187151
6.32000000000000	0.999999712106665
6.36000000000000	0.999999765848783
6.40000000000000	0.999999809639474
6.44000000000000	0.999999845303023
6.48000000000000	0.999999874333427
6.52000000000000	0.999999897953251
6.56000000000000	0.999999917162247
6.60000000000000	0.999999932777451
6.64000000000001	0.999999945466076
6.68000000000001	0.999999955772672
6.72000000000001	0.999999964141395
6.76000000000001	0.999999970934336
6.80000000000001	0.999999976446461
6.84000000000001	0.999999980917960
6.88000000000001	0.999999984544338
6.92000000000001	0.999999987484593
6.96000000000001	0.999999989868010
7.00000000000001	0.999999991799680
7.04000000000001	0.999999993364947
7.08000000000001	0.999999994633119
7.12000000000001	0.999999995660471
7.16000000000001	0.999999996492647
7.20000000000001	0.999999997166672
7.24000000000001	0.999999997712703
7.28000000000001	0.999999998154732
7.32000000000001	0.999999998512823
7.36000000000001	0.999999998802866
7.40000000000001	0.999999999037799
7.44000000000001	0.999999999228102
7.48000000000001	0.999999999382288
7.52000000000001	0.999999999507225
7.56000000000001	0.999999999608469

```
   7.60000000000001       0.999999999690545
   7.64000000000001       0.999999999757094
   7.68000000000001       0.999999999811067
   7.72000000000001       0.999999999854846
   7.76000000000001       0.999999999890381
   7.80000000000001       0.999999999919232
   7.84000000000001       0.999999999942655
   7.88000000000001       0.999999999961695
   7.92000000000001       0.999999999977173
   7.96000000000001       0.999999999989755
   8.00000000000001        1.00000000000000

! Output from mfd version 1.01
! For probability of flaw =  0.13718317
! argument in( 1) =     10.00000
! argument in( 2) =      0.76000
! argument in( 3) =      5.00000
! argument in( 4) =      3.00000
! argument in( 5) =      0.00340
! argument in( 6) =      3.00000
! argument in( 7) =      4.00000
```

4. REFERENCES

CRWMS M&O 1999f. *Testing of Software Routine to Determine Deviate and Cumulative Probability: ModStandardNormal Version 1.0*. CAL-EBS-MD-000004 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991018.0213.

CRWMS M&O 2000g. *Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis.* CAL-EBS-PA-000003 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC

Press, W.H.; Teukolsky, S.A.; Vetterling, W.T.; and Flannery, B.P. 1992. *Numerical Recipes in Fortran 77*, *The Art of Scientific Computing.* Volume 1 of *Fortran Numerical Recipes.* 2nd edition. Cambridge, United Kingdom: Cambridge University Press. TIC: 243606.

ATTACHMENT III

SCCD SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Name and Version Number: SCCD (Stress Corrosion Cracking Dissolution), version 1.01

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 5.0, Standard Edition.

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

2. DESCRIPTION AND TESTING

The software routine SCCD calculates the hoop stress and hoop stress intensity versus depth resulting from a stress corrosion cracking event. The hoop stress and hoop stress intensity tables are calculated for a user-specified number of angles (in the range 0 to pi radians) around the waste package. Uncertainty is included via an input standard normal random number that describes the deviation from the median yield stress range. Variability is included via the input amplitude for the angular variation of hoop stress. These calculations are based on the abstraction of hoop stress versus corrosion stress as discussed in the Stress Corrosion Cracking AMR (CRWMS M&O 2000h). The outputs of SCCD are:

- A text file in WAPDEG table format for the user specified number of angles of tables for hoop stress versus depth, and
- A text file in WAPDEG table format for the user specified number of angles of tables for hoop stress intensity versus depth.

2.1 DESCRIPTION OF SOFTWARE ROUTINE AND THE EXECUTION ENVIRONMENT

SCCD is a FORTRAN program 308 lines in length. It conforms to the FORTRAN 90 standard and is thus highly portable. SCCD was developed and tested in the Windows NT 4.0 operating system, and has been compiled with Digital FORTRAN 5.0 in the Windows NT 4.0 environment. SCCD is designed to be compiled as a DLL (SCCD.dll) and be executed within GoldSim, with input parameters specified by inserting them as data elements in the GoldSim (Golder Associates 2000) environment. SCCD was developed to run with GoldSim to determine the stresses at various angles around the waste package closure lid circumference. The output stress tables are used by the WAPDEG DLL in GoldSim to generate distributions for waste package failures and consequent dose.

WAPDEG tables are formatted so that lines proceeded by a “!” are comment lines. The first line proceeded by a “#” contains two numbers, where the first number indicates the number of tables, each table containing the number of columns specified by the second number. The next line proceeded by a “#” contains a number that specifies the number of rows in the lookup table. The next line proceeded by a “#” with a fraction indicates that this lookup table corresponds to that fraction of the waste packages/drip shields to be simulated. This is followed by one more comment line (proceeded by a “!”) which is used to specify column headers. The subsequent rows consist of the first table, with subsequent tables preceded by the latter three line entries of number of rows, fraction applied, and header line.

Compilation of SCCD requires the module modDefaultSize.f to be present from the WAPDEG library (CRWMS M&O 1999f).

The bulk of SCCD’s coding is devoted to computing and scaling the hoop stress and hoop stress intensity at various angles from a corrosion event, given the stress intensity versus depth at the event (i.e., the stress intensity versus depth at zero angle). The inputs are read as part of the argument list of SCCD, as the elements of array in(*):

in(1)	z	Uncertain deviation from median yield stress range (sampled from N(0,1))
in(2)	sinf	Sine of fracture angle
in(3)	a(1)	Zero order regression coefficient from model abstraction for stress vs. depth at zero degrees
in(4)	a(2)	First order regression coefficient from model abstraction for stress vs. depth at zero degrees
in(5)	a(3)	Second order regression coefficient from model abstraction for stress vs. depth at zero degrees
in(6)	a(4)	Third order regression coefficient from model abstraction for stress vs. depth at zero degrees
in(7)	nangle	number of angles in the range zero to π radians to compute tables of stress and KI versus depth
in(8)	ys	Expected yield strength [MPa]
in(9)	fys	Fraction yield strength range
in(10)	amp	Angular amplitude for the equation of angular variation of stress [MPa]
in(11)	idxinp	File index for input table of stress intensity vs. depth
in(12)	idxkin	File index for output hoop stress intensity vs. depth at nangle angles
in(13)	idxstr	File index for output hoop stress vs. depth at nangle angles

The first output table file consists of nangle tables of stress intensity versus depth, written to the file referenced by index in(12). The second output table file consists of nangle tables of stress versus depth, written to the file referenced by index in(13). Like all GoldSim DLL’s, the project coding standards require all DLL’s to accept as input a ‘method’ variable, which controls the operation of the program (see Figure I-1). If a DLL is called with the following values of ‘method’, the following will occur:

Method = 0 the DLL is initialized (SCCD requires no initialization, thus nothing happens).

Method = 1	run the DLL's calculations (for SCCD, compute the stress tables and stress intensity tables).
Method = 2	the DLL returns the version number as out(1).
Method = 3	report the number of input and output arguments as out(1) and out(2), respectively (for SCCD, this should yield the values 13 and 1, respectively).
Method = 99	the DLL closes all files and processes.

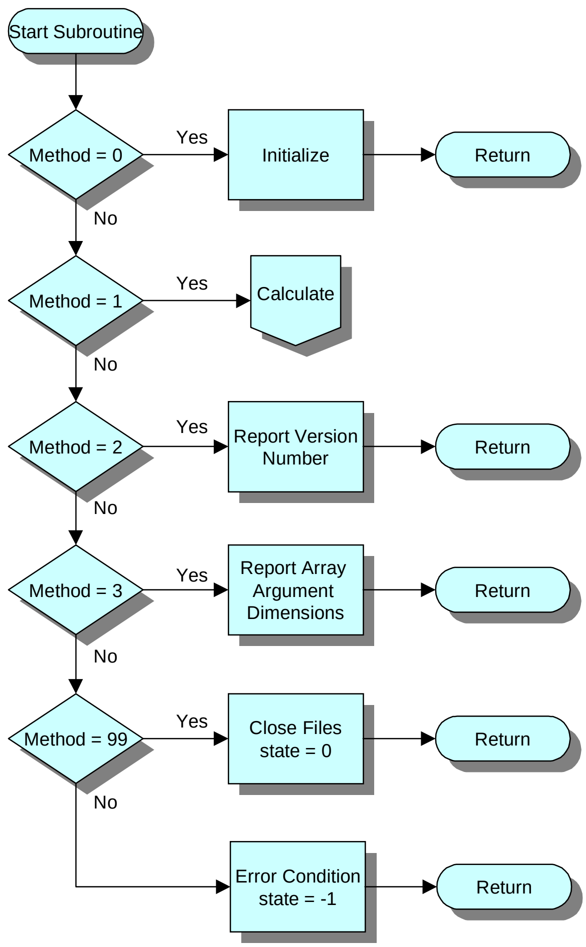


Figure 1. Method calling structure for DLLs in GoldSim

2.2 DESCRIPTION OF THE ALGORITHM

SCCD receives the input parameters from the argument list, and then follows the algorithm presented in the upstream analysis (CRWMS M&O 2000h) and Sections 4.1.8 and 4.1.9 of this report. Specifically, the following steps are performed:

1. Read from an external file the stress intensity factor versus depth at zero angle

   kin, depth *nrows* values of stress intensity factor K_I and depth.

2. Based on the equation for stress versus depth at zero angle (see Equation (5), Section 4.1.8 of this report) and the input look-up table for the stress intensity factor versus depth at zero angle (see Table 6, Section 4.1.8 of this report),
   a. calculate stress and stress intensity factor versus depth at each of the *nangle* angles
   b. re-scale, to account for uncertainty, the output tables from (a), above, to the yield stress (*ys*) range using the random deviate *z* (see Equation 8 of this report).
3. Output:
   a. stress intensity factor versus depth for *nangle* angles
   b. stress versus depth for *nangle* angles

2.3 DESCRIPTION OF TEST CASES

The testing approach involves comparing the results of SCCD with the example calculations presented in the Mathcad worksheets associated with the Stress Corrosion Cracking AMR (CRWMS M&O 2000h). The specific test cases calculate, for various angles, the hoop stress and hoop stress intensity versus depth, given a random deviate, *z*, and a table of stress intensity versus depth at zero angle. The output tables are checked to match the results for the test cases evaluated for two set of calculations, one set of test runs to evaluate the (10 mm) Alloy 22 inner lid, and a second set of test runs to evaluate the (25 mm) Alloy 22 outer lid.

2.3.1 Alloy 22 Inner Lid Test Case

Running in the GoldSim environment as a DLL creates the first fourteen test files (seven executions), where the following values are inserted as data elements in the SCCD input stream with values for in(1), in(12), and in(13) varied as indicated.

z	in(1) =	0, 1, -1, 2, -2, 3, -3
sinf	in(2) =	0.60887
a(1)	in(3) =	-437.72054
a(2)	in(4) =	176.96724
a(3)	in(5) =	-15.60607
a(4)	in(6) =	0.36710
nangle	in(7) =	1
ys	in(8) =	322.12305
fys	in(9) =	0.05
amp	in(10) =	17.23689

The remaining inputs are indices of the locations within the GoldSim file for output filenames

inputidx	in(11) =	1
outputidxk	in(12) =	10, 11, 12, 13, 14, 15, 16
outputidxs	in(13) =	3, 4, 5, 6, 7, 8, 9

The last test run is produced with the following input stream where in(7) = 3:

z	in(1) =	0
sinf	in(2) =	0.60887
a(1)	in(3) =	-437.72054
a(2)	in(4) =	176.96724
a(3)	in(5) =	-15.60607
a(4)	in(6) =	0.36710
nangle	in(7) =	3.00000
ys	in(8) =	322.12305
fys	in(9) =	0.05
amp	in(10) =	17.23689
inputidx	in(11) =	1.00000
outputidxk	in(12) =	18.00000
outputidxs	in(13) =	17.00000

The test case requires as input a text file WD4DLL.wap, which is a list of filenames to be read by SCCD. The names of files used by SCCD for the input and output tables are found in this file by their line index. The input table of stress intensity versus depth at the zero angle, KIinM.fil, is given in Section 3.0 of this SRR. Each execution of the routine produces two output files, which are the resulting tables of stress intensity versus depth and stress versus depth, respectively.

2.3.2 Alloy 22 Outer Lid Test Case

Running in the GoldSim environment as a DLL creates the first fourteen test files (seven executions), where the following values are inserted as data elements in the SCCD input stream with values for in(1), in(12), and in(13) varied as indicated.

z	in(1) =	0, 1, -1, 2, -2, 3, -3
sinf	in(2) =	1.0
a(1)	in(3) =	-356.26778
a(2)	in(4) =	37.18077
a(3)	in(5) =	1.43639
a(4)	in(6) =	-0.06528
nangle	in(7) =	1
ys	in(8) =	322.12305
fys	in(9) =	0.05
amp	in(10) =	17.23689

The remaining inputs are indices of the locations within the WD4DLL.wap file for input and output filenames

inputidx	in(11) =	2
outputidxk	in(12) =	19, 20, 21, 22, 23, 24, 25
outputidxs	in(13) =	26, 27, 28, 29, 30, 31, 32

The last test run is produced with the following input stream where in(7) = 3:

z	in(1) =	0.00000
sinf	in(2) =	1.00000
a(1)	in(3) =	-356.26778
a(2)	in(4) =	37.18077
a(3)	in(5) =	1.43639
a(4)	in(6) =	-0.06528
nangle	in(7) =	3.00000
ys	in(8) =	322.12305
fys	in(9) =	0.05
amp	in(10) =	17.23689
inputidx	in(11) =	2.00000
outputidxk	in(12) =	34.00000
outputidxs	in(13) =	33.00000

The test case requires as input a text file WD4DLL.wap, which is a list of filenames to be read by SCCD. The names of files used by SCCD for the input and output tables are found in this file by their line index. The input table of stress intensity versus depth at zero angle, KIinO.fil, is given in Section 3.0 of this SRR. Each execution of the routine produces two output files, which are the resulting tables of stress intensity versus depth and stress versus depth, respectively.

2.4 DESCRIPTION OF TEST RESULTS

The test results for the Alloy 22 inner lid test case should be compared to the results of the output file, data10.txt, form the Mathcad worksheet “Hoop Stress and Stress Intensity Calculation (10mm Lid)” (see Section 3.3). The test results for the Alloy 22 outer lid test case should be compared to the output file, data25.txt, from the Mathcad worksheet “Hoop Stress and Stress Intensity Calculation (25mm Lid)” (see Section 3.3). Visual comparison of the test case output files with the appropriate rows and columns of the above-named worksheets confirms that SCCD gives the anticipated results (DTN: MO0002SPASDA04.001). The output tables match the results for these cases, thus the tests are considered successful.

2.5 RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED

The preceding test cases evaluate SCCD for a typical set of parameters as observed from the study of stress corrosion cracking discussed in the Stress Corrosion Cracking AMR (CRWMS M&O 2000h). SCCD will execute properly if the following ranges and types of parameter values are met:

Variable	Range	Description
z	real	Uncertain deviation from median yield stress range
sinf	real [0,1]	sine of fracture angle
0 order regression coefficient	real	Regression coefficient from model abstraction for stress v. Depth at 0 degrees
1 order regression coefficient	real	Regression coefficient from model abstraction for stress v. Depth at 0 degrees
2 order regression coefficient	real	Regression coefficient from model abstraction for stress v. Depth at 0 degrees
3 order regression coefficient	real	Regression coefficient from model abstraction for stress v. Depth at 0 degrees
Number of angles	positive integer	Divisions of the range 0 to π radians to compute tables of stress and KI versus depth
Yield strength	positive real	Expected yield strength
Fraction yield stress range	real [0,1]	Fraction of yield strength range
Amplitude	real	Angular amplitude for the equation of angular variation of stress
File index 1	integer	File index for input table of stress intensity vs. depth
File index 2	integer	File index for output stress intensity vs. depth at various angles
File index 3	integer	File index for output stress vs. depth at various angles

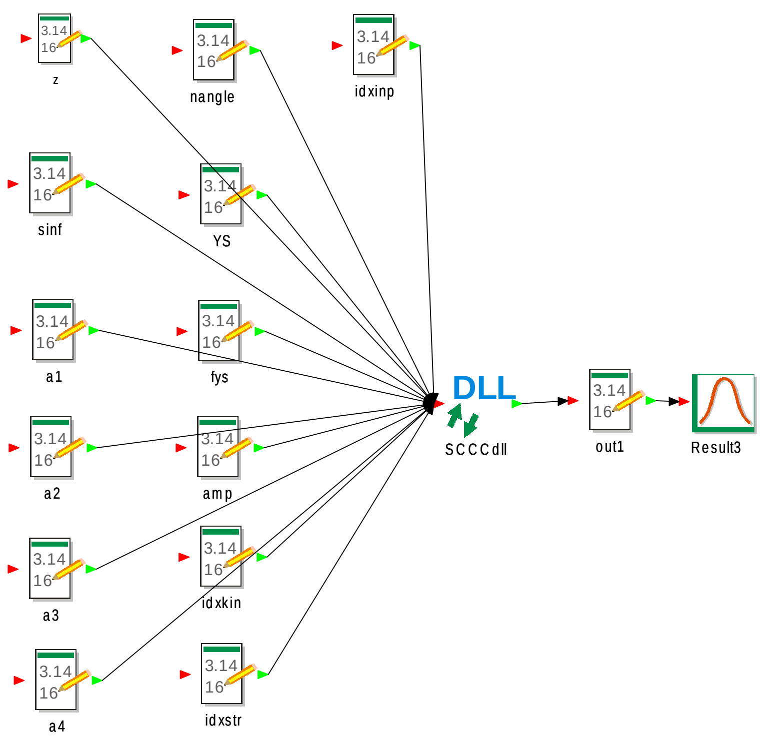


Figure 2 Representative GoldSim SCCD Container Element

2.6 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

None

3. SUPPORTING INFORMATION

3.1 DIRECTORY LISTING OF EXECUTABLE AND DATA FILES

```
Directory of SRRdir

Program files:
02/04/00  11:10a                 12,288 SCCD.dll
04/12/00  10:18a                606,130 SCCDtestv2.gsm

Mathcad files:
04/11/00  04:44p                 23,541 SCCD_10revC.mcd
04/11/00  04:49p                 22,857 SCCD_25revC.mcd
04/12/00  09:43a                 16,900 data10.txt
04/12/00  09:44a                 16,900 data25.txt

Input files:
02/10/00  01:57p                    586 WD4DLL.wap
01/14/00  02:06p                  1,436 WDKIinM.fil
01/14/00  09:26p                  1,439 WDKIinO.fil

Output files:
04/12/00  10:17a                  3,126 WDdata10c01.fil
04/12/00  10:17a                  3,126 WDdata10c02.fil
04/12/00  10:17a                  3,126 WDdata10c03.fil
04/12/00  10:17a                  3,126 WDdata10c04.fil
04/12/00  10:17a                  3,126 WDdata10c05.fil
04/12/00  10:17a                  3,126 WDdata10c06.fil
04/12/00  10:17a                  3,126 WDdata10c07.fil
04/12/00  10:17a                  3,136 WDdata10c08.fil
04/12/00  10:17a                  3,136 WDdata10c09.fil
04/12/00  10:17a                  3,136 WDdata10c10.fil
04/12/00  10:17a                  3,136 WDdata10c11.fil
04/12/00  10:17a                  3,136 WDdata10c12.fil
04/12/00  10:17a                  3,136 WDdata10c13.fil
04/12/00  10:17a                  3,136 WDdata10c14.fil
04/12/00  10:17a                  8,270 WDdata10c15to17.fil
04/12/00  10:17a                  8,280 WDdata10c18to20.fil
04/12/00  10:17a                  3,126 WDdata25c01.fil
04/12/00  10:17a                  3,126 WDdata25c02.fil
04/12/00  10:17a                  3,126 WDdata25c03.fil
04/12/00  10:17a                  3,126 WDdata25c04.fil
04/12/00  10:17a                  3,126 WDdata25c05.fil
04/12/00  10:17a                  3,126 WDdata25c06.fil
04/12/00  10:17a                  3,126 WDdata25c07.fil
04/12/00  10:17a                  3,136 WDdata25c08.fil
04/12/00  10:17a                  3,136 WDdata25c09.fil
04/12/00  10:17a                  3,136 WDdata25c10.fil
04/12/00  10:17a                  3,136 WDdata25c11.fil
04/12/00  10:17a                  3,136 WDdata25c12.fil
04/12/00  10:17a                  3,136 WDdata25c13.fil
04/12/00  10:17a                  3,136 WDdata25c14.fil
04/12/00  10:17a                  8,270 WDdata25c15to17.fil
04/12/00  10:17a                  8,280 WDdata25c18to20.fil
```

3.2 COMPUTER LISTING OF SOURCE CODE

```
subroutine sccd(method, state, in, out)
!
!  Subroutine to calculate stress vs. depth and stress intensity
!  vs depth for n tables corresponding to n angles from 0 to pi.
!
!  1. From argument list:
!     z              a deviate of a standard normal.
!     sinf           sin of fracture angle.
!     a(1),...,a(4) coeffecients for stress vs. depth equation
!     nangle         number of angles to calculate tables
!     ys             yield stress
!     fys            fraction of yeild stress range
!     amp            angular amplitude
!     idxinp       integer location of input file name for KI
!     idxkin     integer location of output file name for k v. depth
!     idxstr     integer location of output file name for s v. depth
!  2. Read from external table\file:
!        kin       nrows values of stress intensity KI
!        depth     nrows values of depth, corresponding to KI.
!  3. Calculate:
!     a. calculate hoop stress and hoop stress intensity vs. depth at
!        nangle's
!     b. rescale tables to YS range for RV z.
!  4. Output:
!     a. ki vs. depth for nangle's
!     b. stress vs. depth for nangles's
!
!DEC$ ATTRIBUTES dllexport,c :: sccd
!DEC$ ATTRIBUTES value       :: method
!DEC$ ATTRIBUTES reference   :: state
!DEC$ ATTRIBUTES reference   :: in
!DEC$ ATTRIBUTES reference   :: out
      USE ModDefaultsize
      IMPLICIT NONE
      integer(IKind) method   ! input, tells sccd what to do
      integer(IKind) state    ! return, 0 = OK
      real(RKind)    in(*)    ! input arguments
      real(RKind)    out(*)   ! output arguments
      real(RKind),PARAMETER :: VERSION = 1.01
      integer(IKind),PARAMETER :: NUMIN = 13, NUMOUT = 1
      real(RKind),PARAMETER :: PI = 3.141592653589793
      integer(IKind) :: kinunit , strunit, errunit
      integer(IKind) :: idxinp, idxkin, idxstr
      character(LEN = 80) :: inptab, kintab, strtab, line1
      real(RKind), ALLOCATABLE, DIMENSION(:) :: kin
      real(RKind), ALLOCATABLE, DIMENSION(:) :: depth
      real(RKind) a(4)
      integer(IKind) n, i, j, nangle, nrows, nsets, ncol
      real(RKind) ys, fys, amp, angle, dangle, rscale, ki, z, thick
      real(RKind) str, strta, strt0, sinf
      logical(LKind) :: OK
!
!*********************************************************************
!
      if (method .eq. 0) then        ! Initialize
        state = 0
```

```
        return
      elseif (method .eq. 2) then    ! Report code version
        out(1) = VERSION
        state = 0
        return
      elseif (method .eq. 3) then    ! Report number of arguments
        out(1) = NUMIN
        out(2) = NUMOUT
        state = 0
        return
      elseif (method .eq. 1) then    ! Calculate
        z      = in(1)
        sinf   = in(2)
        a(1)   = in(3)
        a(2)   = in(4)
        a(3)   = in(5)
        a(4)   = in(6)
        nangle = in(7)
        ys     = in(8)
        fys    = in(9)
        amp    = in(10)
        idxinp = in(11)
        idxkin = in(12)
        idxstr = in(13)
        out(1) = z
        if (nangle .le. 1) then
          nangle = 1
          dangle = 0.
        else
          dangle = PI/(nangle - 1)  !delta angle increment
        end if
!
!  Open the file list and find the I/O filenames
!
        kinunit = nextfreeunit()
        open(unit = kinunit, file = 'WD4DLL.wap')
        n = max(idxinp, idxkin, idxstr)
        do i = 1, n
           read(kinunit,*) line1
           if (i .eq. idxinp) inptab = line1
           if (i .eq. idxkin) kintab = line1
           if (i .eq. idxstr) strtab = line1
        end do
        close(unit = kinunit)
!
!  Open Input KI vs. Depth table and read contents
!  Read in values for: nrows, ncol, kin(1:nrows), depth(1:nrows)
!  Mainly dealing with file formating here.
!
        inquire(file = inptab, exist = OK)
        if (.not. OK) then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit,file = 'sccderror.log')
          write(errunit,*) 'input file not found'
          close(unit = errunit)
          return
```

```
        end if
        kinunit = nextfreeunit()
        open(kinunit, file = inptab)
!  Scroll through the preliminary comments
        line1 = '!'
        do while (line1(1:1) .eq. '!' .or. line1(1:1) .eq. ' ')
          read(kinunit, 9000) line1
 9000     format(a80)
        end do
!  First noncomment line must be #-character, then
!  number of data sets (nsets), number of columns (ncols).
        if (line1(1:1) .ne. '#') then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit,file = 'sccderror.log')
          write(errunit,*) 'format error in input file, 123'
          close(unit = errunit)
          return
        end if
        read(line1(2: 79), *) nsets, ncol
        if (nsets .le. 0) then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit, file = 'sccderror.log')
          write(errunit,*) 'nsets = 0 in input file'
          close(unit = errunit)
          return
        end if
        if (ncol .lt. 2) then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit,file = 'sccderror.log')
          write(errunit,*) 'ncol < 2 in input file'
          close(unit = errunit)
          return
        end if
!  Read the number of rows (nrows) (begins the set)
        read(kinunit, 9000) line1
        if (line1(1:1) .ne. '#') then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit, file = 'sccderror.log')
          write(errunit,*) 'format error in input file, 147'
          close(unit = errunit)
          return
        end if
        read(line1(2:79), *) nrows
        if (nrows .le. 0) then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit, file = 'sccderror.log')
          write(errunit,*) 'error, number of rows in input file'
          close(unit = errunit)
          return
        end if
!  Read the fraction and discard
        read(kinunit, 9000) line1
```

```
        if (line1(1:1) .ne. '#') then
          state = 1
          errunit = nextfreeunit()
          open(unit = errunit,file = 'sccderror.log')
          write(errunit,*) 'format error in input file, 164'
          close(unit = errunit)
          return
        end if
!  Read the column header and discard
        read(kinunit, 9000) line1       !Column header line
!  Read the nrows rows in the set
        ALLOCATE(depth(nrows))
        ALLOCATE(kin(nrows))
        do j = 1, nrows
          read(kinunit,*) kin(j), depth(j)
        end do
        close(kinunit)
!
!  Write headers to output files*******
!
        kinunit = nextfreeunit()
        open(kinunit, file = kintab)
        strunit = nextfreeunit()
        open(strunit, file = strtab)
        write(kinunit,3330) VERSION
        write(kinunit,3331) out(1)
        write(kinunit,3334) !title3334
        write(kinunit,3338) ( i, in(i), i = 1, NUMIN )
        write(kinunit,3332) nangle, ncol
        write(strunit,3330) VERSION
        write(strunit,3331) out(1)
        write(strunit,3335) !title3335
        write(strunit,3338) ( i, in(i), i = 1, NUMIN )
        write(strunit,3332) nangle, ncol
 3330   format('! Output from sccd version ',F4.2)
 3331   format('! For sampled random variable z =',F9.5)
 3332   format('#',1x,I5,I5)
 3333   format('#',1x,F9.5)
 3334   format('! Stress Intensity vs. Depth ')
 3335   format('! Stress vs. Depth ')
 3336   format('! KI vs. Depth       (angle = ',f9.5,' radians)')
 3337   format('! Stress vs. Depth   (angle = ',f9.5,' radians)')
 3338   format('! argument in(',I2,') = ',f12.5)
!
! Perform Calculations**************************************************
!   For nangle's from 0 to pi, calculate:
!   scaled stress table  str(depth,angle)*rscale
!   scaled ki table      ki(depth,angle)*rscale
!
        thick = depth(nrows)
        angle = 0.0_RKind
        do i = 1, nangle
          write(kinunit,3332) nrows
          write(kinunit,3333) 1.0/nangle
          write(kinunit,3336) angle
          write(strunit,3332) nrows
          write(strunit,3333) 1.0/nangle
```

```
          write(strunit,3337) angle
          strta = stress(a,amp,thick,angle)
          strt0 = stress(a,amp,thick,0.0_RKind)
          rscale = (strta + ((z*ys*fys)/3.0))/strta
          do j = 1, nrows
            ki = kin(j)*(strta/strt0)*rscale
            str  = stress(a,amp,depth(j),angle)*rscale
            write(kinunit,*) ki,  depth(j)*sinf
            write(strunit,*) str, depth(j)*sinf
          end do !over depths
          angle = angle + dangle
        end do !over angles
        close(unit = kinunit)
        close(unit = strunit)
        DEALLOCATE(depth, kin)
        state = 0
        return
      elseif (method .eq. 99) then   ! Shut-down
        close(unit = kinunit)
        close(unit = strunit)
        close(unit = errunit)
        state = 0
        return
      else
        errunit = nextfreeunit()
        open(unit = errunit,file = 'sccderror.log')
        write(errunit,*) 'sccd crashed method = ',method
        close(unit = errunit)
        state = 1
        return
      end if                         ! end block for method
      CONTAINS     !stress, nextfreeunit
!
! **********************************************************************
!
      real(RKind) FUNCTION stress(a, amp, x, angle)
!
!  Regression equation for stress v. depth abstracted
!  from the finite element code, adapted to angular variation
!  Input : a(*)     array of coefficients
!          amp      amplitude in MPa
!          x        depth in mm
!          angle    angle in radians
!  Output: (function value)
!
      real(RKind) :: a(*), amp, x, angle
!
      stress = a(1)+x*(a(2)+x*(a(3)+x*a(4)))-amp*(1.0-cos(angle))
      return
      END FUNCTION stress
!
!**********************************************************************
!
      integer(IKind) FUNCTION nextfreeunit()
!
!  Find the smallest unit number not currently attached and in use.
!  Avoid units 5 and 6.
```

```
!  Input : (none)
!  Output: (function value)
!  Local : i, InUse
!
!  Local variables
!
      integer(IKind) :: i
      logical InUse
!
      InUse = .true.
      i = 0
      do while (InUse)
        i = i + 1
        if(i .ne. 5 .and. i .ne. 6) then
          inquire(i, opened = InUse)
        end if
      end do
      nextfreeunit = i
      RETURN
      END FUNCTION nextfreeunit
!
!**********************************************************************
!
      END SUBROUTINE sccd
```

3.3 LISTING OF MATHCAD WORKSHEETS

Hoop Stress and Stress Intensity Calculation (10mm Lid)

Conversion Factors: 1 in = 25.4 mm, 1 ksi = 6.89 MPa, 1 ksi-in^½ = 1.0988 MPa-m^½

$c0 := 25.4$

$c1 := 6.894757$

$c2 := 1.098843$

Coefficients for stress from third order polynomial fit from results of finite element code (Ansys 5.4).

$A_0 := -63.486 c1$

$A_0 = -437.720543$

$A_1 := 651.94 \frac{c1}{c0}$

$A_1 = 176.967239$

$A_2 := -1460.3 \frac{c1}{c0 \cdot c0}$

$A_2 = -15.606072$

$A_3 := 872.5 \frac{c1}{c0 \cdot c0 \cdot c0}$

$A_3 = 0.367099$

$\sigma_s(x) := \left[A_0 + x \cdot \left[A_1 + x \cdot \left(A_2 + x \cdot A_3 \right) \right] \right]$

Stress Intensity Table based on PC-crack calculation given input of radial stress

at 50 linearly spaced points out to (99.97% of length along crack) 16.42 mm.

$$
\mathrm{Ktable} := \begin{pmatrix}
-7.201806034 & 0.3277 \\
-10.05117186 & 0.6579 \\
-12.14661052 & 0.9855 \\
-13.83718048 & 1.3132 \\
-15.26051182 & 1.6408 \\
-16.48813922 & 1.971 \\
-17.60873931 & 2.2987 \\
-18.62418012 & 2.6264 \\
-19.34568044 & 2.954 \\
-18.27353932 & 3.2842 \\
-17.05876838 & 3.6119 \\
-15.73543176 & 3.9395 \\
-14.40693057 & 4.2697 \\
-13.09502192 & 4.5974 \\
-11.74410433 & 4.9251 \\
-10.37129779 & 5.2527 \\
-8.992063026 & 5.5829 \\
-7.619959749 & 5.9106 \\
-6.28349195 & 6.2382 \\
-5.021547684 & 6.5659 \\
-3.791766552 & 6.8961 \\
-2.602642611 & 7.2238 \\
-1.461856773 & 7.5514 \\
-0.376262524 & 7.8791 \\
0.6479086 & 8.2093 \\
1.602739435 & 8.5369 \\
2.489890331 & 8.8646 \\
3.304704392 & 9.1948 \\
4.043027992 & 9.5225 \\
4.701256926 & 9.8501 \\
5.276226526 & 10.1778 \\
5.809253288 & 10.508 \\
6.267459831 & 10.8356 \\
6.633989902 & 11.1633 \\
6.907239191 & 11.491 \\
7.086141819 & 11.8212 \\
7.170016506 & 12.1488 \\
7.171796631 & 12.4765 \\
7.082153019 & 12.8067 \\
6.8851964 & 13.1343 \\
6.581695963 & 13.462 \\
6.173014275 & 13.7897 \\
5.661052333 & 14.1199 \\
5.214086954 & 14.4475 \\
5.185517036 & 14.7752 \\
5.092620849 & 15.1028 \\
4.940639873 & 15.433 \\
4.735255128 & 15.7607 \\
4.482741007 & 16.0884 \\
4.18995429 & 16.4186
\end{pmatrix}
$$

$\text{Thck} := \text{Ktable}_{49,1}$

$\text{Thck} = 16.4186$

$K_s(x) := \text{linterp}\left(\text{Ktable}^{\langle 1\rangle}, \text{Ktable}^{\langle 0\rangle}, x\right)$

Functional form based on angular variation.

$\sigma_t(x,\theta) := \sigma_s(x) - (c1 \cdot 2.5)\cdot(1-\cos(\theta))$

$$K_t(x,\theta) := K_s(x)\cdot\left(\frac{\sigma_t(\text{Thck},\theta)}{\sigma_t(\text{Thck},0)}\right)$$

Rescaling based on uncertainty in range of Yield Stress (46.72 ksi).

$\text{YS} := c1 \cdot 46.72$

$\text{YS} = 322.123047$

$F := 0.05$

$$\text{rscale}(\theta,s) := \left(\frac{\sigma_t(\text{Thck},\theta) + s\cdot\frac{\text{YS}\,F}{3}}{\sigma_t(\text{Thck},\theta)}\right)$$

$\sigma_u(x,\theta,s) := \overrightarrow{\left(\sigma_t(x,\theta)\cdot\text{rscale}(\theta,s)\right)}$

$K_u(x,\theta,s) := \overrightarrow{\left(K_t(x,\theta)\cdot\text{rscale}(\theta,s)\right)}$

$$\text{sinf} := \frac{20.256 - 19.764}{\sqrt{(20.256-19.764)^2 + (30.641-30.0)^2}}$$

$\text{sinf} = 0.60887312121$

$\text{asin}(\text{sinf}) = 37.508067\,\text{deg}$

$\text{xx} := \text{Ktable}^{\langle 1\rangle}$

$\text{data10}^{\langle 0\rangle} := \text{Ktable}^{\langle 1\rangle}\cdot\text{sinf}$

$\text{data10}^{\langle 1\rangle} := \sigma_u(\text{xx},0,0)$

$\text{data10}^{\langle 2\rangle} := \sigma_u(\text{xx},0,1)$

$\text{data10}^{\langle 3\rangle} := \sigma_u(\text{xx},0,-1)$

$\text{data10}^{\langle 4\rangle} := \sigma_u(\text{xx},0,2)$

$\text{data10}^{\langle 5\rangle} := \sigma_u(\text{xx},0,-2)$

$\text{data10}^{\langle 6\rangle} := \sigma_u(\text{xx},0,3)$

$\text{data10}^{\langle 7\rangle} := \sigma_u(\text{xx},0,-3)$

$data10^{\langle 8 \rangle} := K_u(xx, 0, 0)$

$data10^{\langle 9 \rangle} := K_u(xx, 0, 1)$

$data10^{\langle 10 \rangle} := K_u(xx, 0, -1)$

$data10^{\langle 11 \rangle} := K_u(xx, 0, 2)$

$data10^{\langle 12 \rangle} := K_u(xx, 0, -2)$

$data10^{\langle 13 \rangle} := K_u(xx, 0, 3)$

$data10^{\langle 14 \rangle} := K_u(xx, 0, -3)$

$data10^{\langle 15 \rangle} := \sigma_u(xx, 0, 0)$

$data10^{\langle 16 \rangle} := \sigma_u\left(xx, \frac{\pi}{2}, 0\right)$

$data10^{\langle 17 \rangle} := \sigma_u(xx, \pi, 0)$

$data10^{\langle 18 \rangle} := K_u(xx, 0, 0)$

$data10^{\langle 19 \rangle} := K_u\left(xx, \frac{\pi}{2}, 0\right)$

$data10^{\langle 20 \rangle} := K_u(xx, \pi, 0)$

WRITEPRN("data10.txt") := data10

Hoop Stress and Stress Intensity Calculation (25mm lid)

Conversion Factors: 1 in = 25.4 mm, 1 ksi = 6.89 MPa, 1 ksi-in^½ = 1.0988 MPa-m^½

$c0 := 25.4$

$c1 := 6.894757$

$c2 := 1.098843$

Coefficients for stress from third order polynomial fit from results of finite element code (Ansys 5.4).

$A_0 := -51.672275 \cdot c1$

$A_0 = -356.26778$

$$A_1 := 136.97241 \cdot \frac{c1}{c0}$$

$A_1 = 37.180767$

$$A_2 := 134.40677 \cdot \frac{c1}{c0 \cdot c0}$$

$A_2 = 1.436391$

$$A_3 := -155.15755 \cdot \frac{c1}{c0 \cdot c0 \cdot c0}$$

$A_3 = -0.065282$

$$\sigma_s(x) := \left[A_0 + x \cdot \left[A_1 + x \cdot \left(A_2 + x \cdot A_3 \right) \right] \right]$$

Stress Intensity Table based on PC-crack calculation given input of radial stress

at 50 linearly spaced points out to (80% of thickness) 0.7872 inches or 19.995 mm.

$$\mathrm{Ktable} := \begin{pmatrix} -8.096912553 & 0.3988 \\ -11.08864448 & 0.8001 \\ -13.12743778 & 1.1989 \\ -14.62395207 & 1.6002 \\ -15.74125563 & 1.999 \\ -16.56494834 & 2.4003 \\ -17.16634511 & 2.7991 \\ -17.5702798 & 3.2004 \\ -17.79521296 & 3.5992 \\ -17.85960516 & 3.998 \\ -17.77785124 & 4.3993 \\ -17.56148906 & 4.7981 \\ -17.22755067 & 5.1994 \\ -16.78515648 & 5.5982 \\ -16.23441637 & 5.9995 \\ -15.58159374 & 6.3983 \\ -14.83251247 & 6.797 \\ -13.99233711 & 7.1984 \\ -13.06249616 & 7.5971 \\ -12.03771518 & 7.9985 \\ -10.93137807 & 8.3972 \\ -9.747286832 & 8.7986 \\ -8.489320377 & 9.1973 \\ -7.161148843 & 9.5987 \\ -5.7664094 & 9.9974 \\ -4.327309665 & 10.3962 \\ -2.830795383 & 10.7975 \\ -1.280437794 & 11.1963 \\ 0.320255595 & 11.5976 \\ 1.967753102 & 11.9964 \\ 3.658542826 & 12.3977 \\ 5.415098304 & 12.7965 \\ 7.218783158 & 13.1978 \\ 9.05768593 & 13.5966 \\ 10.92825736 & 13.9954 \\ 12.82690422 & 14.3967 \\ 14.74987947 & 14.7955 \\ 16.73175271 & 15.1968 \\ 18.7698867 & 15.5956 \\ 20.82285508 & 15.9969 \\ 22.88648224 & 16.3957 \\ 24.95692222 & 16.7945 \\ 27.03021919 & 17.1958 \\ 29.13461342 & 17.5946 \\ 31.33328838 & 17.9959 \\ 33.52559005 & 18.3947 \\ 35.70701317 & 18.796 \\ 37.87294261 & 19.1948 \\ 40.01865333 & 19.5961 \\ 42.13953021 & 19.9949 \end{pmatrix}$$

$\text{Thck} := \text{Ktable}_{49,1}$

$\text{Thck} = 19.9949$

$K_s(x) := \text{linterp}\left(\text{Ktable}^{\langle 1\rangle}, \text{Ktable}^{\langle 0\rangle}, x\right)$

Functional form based on angular variation.

$\sigma_t(x,\theta) := \sigma_s(x) - (c1 \cdot 2.5) \cdot (1 - \cos(\theta))$

$$K_t(x,\theta) := K_s(x) \cdot \left(\frac{\sigma_t(\text{Thck},\theta)}{\sigma_t(\text{Thck},0)}\right)$$

Rescaling based on uncertainty in range of Yield Stress (46.72 ksi).

$\text{YS} := c1 \cdot 46.72$

$\text{YS} = 322.123047$

$F := 0.05$

$$\text{rscale}(\theta, s) := \left(\frac{\sigma_t(\text{Thck},\theta) + s \cdot \frac{\text{YS} \cdot F}{3}}{\sigma_t(\text{Thck},\theta)}\right)$$

$\sigma_u(x,\theta,s) := \overrightarrow{\left(\sigma_t(x,\theta) \cdot \text{rscale}(\theta,s)\right)}$

$K_u(x,\theta,s) := \overrightarrow{\left(K_t(x,\theta) \cdot \text{rscale}(\theta,s)\right)}$

$\text{xx} := \text{Ktable}^{\langle 1\rangle}$

$\text{data25}^{\langle 0\rangle} := \text{Ktable}^{\langle 1\rangle}$

$\text{data25}^{\langle 1\rangle} := \sigma_u(\text{xx}, 0, 0)$

$\text{data25}^{\langle 2\rangle} := \sigma_u(\text{xx}, 0, 1)$

$\text{data25}^{\langle 3\rangle} := \sigma_u(\text{xx}, 0, -1)$

$\text{data25}^{\langle 4\rangle} := \sigma_u(\text{xx}, 0, 2)$

$\text{data25}^{\langle 5\rangle} := \sigma_u(\text{xx}, 0, -2)$

$\text{data25}^{\langle 6\rangle} := \sigma_u(\text{xx}, 0, 3)$

$\text{data25}^{\langle 7\rangle} := \sigma_u(\text{xx}, 0, -3)$

$\text{data25}^{\langle 8\rangle} := K_u(\text{xx}, 0, 0)$

$\text{data25}^{\langle 9\rangle} := K_u(\text{xx}, 0, 1)$

$\text{data25}^{\langle 10\rangle} := K_u(\text{xx}, 0, -1)$

$data25^{\langle 11\rangle} := K_u(xx, 0, 2)$

$data25^{\langle 12\rangle} := K_u(xx, 0, -2)$

$data25^{\langle 13\rangle} := K_u(xx, 0, 3)$

$data25^{\langle 14\rangle} := K_u(xx, 0, -3)$

$data25^{\langle 15\rangle} := \sigma_u(xx, 0, 0)$

$data25^{\langle 16\rangle} := \sigma_u\left(xx, \frac{\pi}{2}, 0\right)$

$data25^{\langle 17\rangle} := \sigma_u(xx, \pi, 0)$

$data25^{\langle 18\rangle} := K_u(xx, 0, 0)$

$data25^{\langle 19\rangle} := K_u\left(xx, \frac{\pi}{2}, 0\right)$

$data25^{\langle 20\rangle} := K_u(xx, \pi, 0)$

WRITEPRN("data25.txt") := data25

3.4 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

Input master file list (WD4DLL.wap).

```
WDKIinM.fil
WDKIinO.fil
WDdata10c01.fil
WDdata10c02.fil
WDdata10c03.fil
WDdata10c04.fil
WDdata10c05.fil
WDdata10c06.fil
WDdata10c07.fil
WDdata10c08.fil
WDdata10c09.fil
WDdata10c10.fil
WDdata10c11.fil
WDdata10c12.fil
WDdata10c13.fil
WDdata10c14.fil
WDdata10c15to17.fil
WDdata10c18to20.fil
WDdata25c01.fil
WDdata25c02.fil
WDdata25c03.fil
WDdata25c04.fil
WDdata25c05.fil
WDdata25c06.fil
```

```
WDdata25c07.fil
WDdata25c08.fil
WDdata25c09.fil
WDdata25c10.fil
WDdata25c11.fil
WDdata25c12.fil
WDdata25c13.fil
WDdata25c14.fil
WDdata25c15to17.fil
WDdata25c18to20.fil
```

Listing of Input Stress Intensity File (KIinM.fil) for (10mm) Middle Lid Test Case

```
! KIinM.fil
! From Thinlid1.xls
! AO30:AO79       A89:A138
#  1  2
#  50
#  1.0
! KI (MPA*m½)     depth (mm)
-7.201806034      0.3277
-10.05117186      0.6579
-12.14661052      0.9855
-13.83718048      1.3132
-15.26051182      1.6408
-16.48813922      1.9710
-17.60873931      2.2987
-18.62418012      2.6264
-19.34568044      2.9540
-18.27353932      3.2842
-17.05876838      3.6119
-15.73543176      3.9395
-14.40693057      4.2697
-13.09502192      4.5974
-11.74410433      4.9251
-10.37129779      5.2527
-8.992063026      5.5829
-7.619959749      5.9106
-6.28349195       6.2382
-5.021547684      6.5659
-3.791766552      6.8961
-2.602642611      7.2238
-1.461856773      7.5514
-0.376262524      7.8791
0.6479086         8.2093
1.602739435       8.5369
2.489890331       8.8646
3.304704392       9.1948
4.043027992       9.5225
4.701256926       9.8501
5.276226526       10.1778
5.809253288       10.5080
6.267459831       10.8356
6.633989902       11.1633
6.907239191       11.4910
7.086141819       11.8212
7.170016506       12.1488
```

```
7.171796631       12.4765
7.082153019       12.8067
6.8851964         13.1343
6.581695963       13.4620
6.173014275       13.7897
5.661052333       14.1199
5.214086954       14.4475
5.185517036       14.7752
5.092620849       15.1028
4.940639873       15.4330
4.735255128       15.7607
4.482741007       16.0884
4.18995429        16.4186
```

Listing of Input Stress Intensity File (KIinM.fil) for (10mm) Inner Lid Test Case

```
! KIinM.fil
! From Thinlid1.xls
! AO30:AO79       A89:A138
#  1  2
#  50
#  1.0
! KI (MPA*m½)     depth (mm)
-7.201806034      0.3277
-10.05117186      0.6579
-12.14661052      0.9855
-13.83718048      1.3132
-15.26051182      1.6408
-16.48813922      1.9710
-17.60873931      2.2987
-18.62418012      2.6264
-19.34568044      2.9540
-18.27353932      3.2842
-17.05876838      3.6119
-15.73543176      3.9395
-14.40693057      4.2697
-13.09502192      4.5974
-11.74410433      4.9251
-10.37129779      5.2527
-8.992063026      5.5829
-7.619959749      5.9106
-6.28349195       6.2382
-5.021547684      6.5659
-3.791766552      6.8961
-2.602642611      7.2238
-1.461856773      7.5514
-0.376262524      7.8791
0.6479086         8.2093
1.602739435       8.5369
2.489890331       8.8646
3.304704392       9.1948
4.043027992       9.5225
4.701256926       9.8501
5.276226526       10.1778
5.809253288       10.5080
```

```
6.267459831       10.8356
6.633989902       11.1633
6.907239191       11.4910
7.086141819       11.8212
7.170016506       12.1488
7.171796631       12.4765
7.082153019       12.8067
6.8851964         13.1343
6.581695963       13.4620
6.173014275       13.7897
5.661052333       14.1199
5.214086954       14.4475
5.185517036       14.7752
5.092620849       15.1028
4.940639873       15.4330
4.735255128       15.7607
4.482741007       16.0884
4.18995429        16.4186
```

Listing of Input Stress Intensity File (KIinO.fil) for (25mm) Outer Lid Test Case

```
! KIinO.fil
! From S&K_OL.xls
! AO29:AO78       A87:A136
#  1  2
#  50
#  1.0
! KI (MPA*m½)     depth (mm)
-8.096912553      0.3988
-11.08864448      0.8001
-13.12743778      1.1989
-14.62395207      1.6002
-15.74125563      1.9990
-16.56494834      2.4003
-17.16634511      2.7991
-17.5702798       3.2004
-17.79521296      3.5992
-17.85960516      3.9980
-17.77785124      4.3993
-17.56148906      4.7981
-17.22755067      5.1994
-16.78515648      5.5982
-16.23441637      5.9995
-15.58159374      6.3983
-14.83251247      6.7970
-13.99233711      7.1984
-13.06249616      7.5971
-12.03771518      7.9985
-10.93137807      8.3972
-9.747286832      8.7986
-8.489320377      9.1973
-7.161148843      9.5987
-5.7664094        9.9974
-4.327309665      10.3962
-2.830795383      10.7975
```

```
-1.280437794      11.1963
0.320255595       11.5976
1.967753102       11.9964
3.658542826       12.3977
5.415098304       12.7965
7.218783158       13.1978
9.05768593        13.5966
10.92825736       13.9954
12.82690422       14.3967
14.74987947       14.7955
16.73175271       15.1968
18.7698867        15.5956
20.82285508       15.9969
22.88648224       16.3957
24.95692222       16.7945
27.03021919       17.1958
29.13461342       17.5946
31.33328838       17.9959
33.52559005       18.3947
35.70701317       18.7960
37.87294261       19.1948
40.01865333       19.5961
42.13953021       19.9949
```

Listing of Output Stress and Stress Intensity Files (WDdata10c15to17.fil and WDdata10c18to20.fil) for (10mm) Inner Lid Test Case

```
! Output from sccd version 1.01
! For sampled random variable z =  0.00000
! Stress Intensity vs. Depth
! argument in( 1) =      0.00000
! argument in( 2) =      0.60887
! argument in( 3) =   -437.72054
! argument in( 4) =    176.96724
! argument in( 5) =    -15.60607
! argument in( 6) =      0.36710
! argument in( 7) =      3.00000
! argument in( 8) =    322.12305
! argument in( 9) =      0.05000
! argument in(10) =     17.23689
! argument in(11) =      1.00000
! argument in(12) =     18.00000
! argument in(13) =     17.00000
#     3    2
#    50
#   0.33333
! KI vs. Depth       (angle =   0.00000 radians)
```

```
! Output from sccd version 1.01
! For sampled random variable z =  0.00000
! Stress vs. Depth
! argument in( 1) =      0.00000
! argument in( 2) =      0.60887
! argument in( 3) =   -437.72054
! argument in( 4) =    176.96724
! argument in( 5) =    -15.60607
! argument in( 6) =      0.36710
! argument in( 7) =      3.00000
! argument in( 8) =    322.12305
! argument in( 9) =      0.05000
! argument in(10) =     17.23689
! argument in(11) =      1.00000
! argument in(12) =     18.00000
! argument in(13) =     17.00000
#     3    2
#    50
#   0.33333
! Stress vs. Depth   (angle =   0.00000 radians)
```

-7.20180603400000	0.199527721820517	-381.391354046354	0.199527721820517
-10.0511718600000	0.400577626444059	-327.944074942598	0.400577626444059
-12.1466105200000	0.600044460952455	-278.124745432091	0.600044460952455
-13.8371804800000	0.799572182772972	-231.408411480447	0.799572182772972
-15.2605118200000	0.999039017281368	-187.746124894520	0.999039017281368
-16.4881392200000	1.20008892190491	-146.734338309176	1.20008892190491
-17.6087393100000	1.39961664372543	-108.929849460936	1.39961664372543
-18.6241801200000	1.59914436554594	-73.9334352802770	1.59914436554594
-19.3456804400000	1.79861120005434	-41.6770222269442	1.79861120005434
-18.2735393200000	1.99966110467788	-11.8475042555369	1.99966110467788
-17.0587683800000	2.19918882649840	15.1711756272377	2.19918882649840
-15.7354317600000	2.39865566100679	39.6852830645551	2.39865566100679
-14.4069305700000	2.59970556563034	61.9467878680317	2.59970556563034
-13.0950219200000	2.79923328745085	81.6887433515208	2.79923328745085
-11.7441043300000	2.99876100927137	99.1663370590975	2.99876100927137
-10.3712977900000	3.19822784377977	114.452739672944	3.19822784377977
-8.99206302600000	3.39927774840331	127.727431624854	3.39927774840331
-7.61995974900000	3.59880547022383	138.862411738665	3.59880547022383
-6.28349195000000	3.79827230473222	148.041130471831	3.79827230473222
-5.02154768400000	3.99780002655274	155.346682805888	3.99780002655274
-3.79176655200000	4.19884993117628	160.888780598165	4.19884993117628
-2.60264261100000	4.39837765299680	164.661508132565	4.39837765299680
-1.46185677300000	4.59784448750519	166.790690751384	4.59784448750519
-0.376262524000000	4.79737220932571	167.355119690056	4.79737220932571
0.647908600000000	4.99842211394925	166.418842014631	4.99842211394925
1.60273943500000	5.19788894845765	164.074962488104	5.19788894845765
2.48989033100000	5.39741667027817	160.398029218561	5.39741667027817
3.30470439200000	5.59846657490171	155.423807439792	5.59846657490171
4.04302799200000	5.79799429672223	149.305623100921	5.79799429672223
4.70125692600000	5.99746113123062	142.090376169171	5.99746113123062
5.27622652600000	6.19698885305114	133.851153100029	6.19698885305114
5.80925328800000	6.39803875767468	124.594011615931	6.39803875767468
6.26745983100000	6.59750559218308	114.540324274169	6.59750559218308
6.63398990200000	6.79703331400359	103.694859700931	6.79703331400359
6.90723919100000	6.99656103582411	92.1380696224587	6.99656103582411
7.08614181900000	7.19761094044765	79.8522271249622	7.19761094044765
7.17001650600000	7.39707777495605	67.1053410871005	7.39707777495605
7.17179663100000	7.59660549677657	53.8764203100514	7.59660549677657
7.08215301900000	7.79765540140011	40.1414657033600	7.79765540140011
6.88519640000000	7.99712223590850	26.1907609908213	7.99712223590850
6.58169596300000	8.19664995772902	11.9907194137937	8.19664995772902
6.17301427500000	8.39617767954954	-2.37693477679909	8.39617767954954
5.66105233300000	8.59722758417308	-16.9451346345174	8.59722758417308

```
   5.21408695400000       8.79669441868148         -31.4108693340314       8.79669441868148
   5.18551703600000       8.99622214050199         -45.8155335190830       8.99622214050199
   5.09262084900000       9.19568897501039         -60.0728759766058       9.19568897501039
   4.94063987300000       9.39673887963393         -74.2201822011426       9.39673887963393
   4.73525512800000       9.59626660145445         -87.9608464820539       9.59626660145445
   4.48274100700000       9.79579432327496         -101.325410484862       9.79579432327496
   4.18995429000000       9.99684422789851         -114.332917016722       9.99684422789851
#    50                                            #    50
#   0.33333                                        #   0.33333
! KI vs. Depth       (angle =   1.57080 radians)   ! Stress vs. Depth   (angle =   1.57080 radians)
  -8.28755421267853      0.199527721820517         -398.628246546354      0.199527721820517
  -11.5664919740185      0.400577626444059         -345.180967442598      0.400577626444059
  -13.9778401014336      0.600044460952455         -295.361637932091      0.600044460952455
  -15.9232813043319      0.799572182772972         -248.645303980447      0.799572182772972
  -17.5611948481243      0.999039017281368         -204.983017394520      0.999039017281368
  -18.9739000199156       1.20008892190491         -163.971230809176       1.20008892190491
  -20.2634423864780       1.39961664372543         -126.166741960936       1.39961664372543
  -21.4319716030261       1.59914436554594         -91.1703277802770       1.59914436554594
  -22.2622457020834       1.79861120005434         -58.9139147269442       1.79861120005434
  -21.0284680060869       1.99966110467788         -29.0843967555369       1.99966110467788
  -19.6305575411692       2.19918882649840         -2.06571687276231       2.19918882649840
  -18.1077139755280       2.39865566100679          22.4483905645551       2.39865566100679
  -16.5789272265161       2.59970556563034          44.7098953680317       2.59970556563034
  -15.0692345178223       2.79923328745085          64.4518508515208       2.79923328745085
  -13.5146518602042       2.99876100927137          81.9294445590975       2.99876100927137
  -11.9348802626275       3.19822784377977          97.2158471729440       3.19822784377977
  -10.3477113185186       3.39927774840331          110.490539124854       3.39927774840331
  -8.76874900825270       3.59880547022383          121.625519238665       3.59880547022383
  -7.23079459995272       3.79827230473222          130.804237971831       3.79827230473222
  -5.77859893285489       3.99780002655274          138.109790305888       3.99780002655274
  -4.36341533126066       4.19884993117628          143.651888098165       4.19884993117628
  -2.99501842080432       4.39837765299680          147.424615632565       4.39837765299680
  -1.68224709193949       4.59784448750519          149.553798251384       4.59784448750519
 -0.432988065927861       4.79737220932571          150.118227190056       4.79737220932571
  0.745587651487789       4.99842211394925          149.181949514631       4.99842211394925
   1.84436930037434       5.19788894845765          146.838069988104       5.19788894845765
   2.86526754599714       5.39741667027817          143.161136718560       5.39741667027817
   3.80292341619275       5.59846657490171          138.186914939792       5.59846657490171
   4.65255708205551       5.79799429672223          132.068730600921       5.79799429672223
   5.41002096668734       5.99746113123062          124.853483669171       5.99746113123062
   6.07167329502636       6.19698885305114          116.614260600029       6.19698885305114
   6.68505946038938       6.39803875767468          107.357119115931       6.39803875767468
   7.21234547000819       6.59750559218308          97.3034317741686       6.59750559218308
```

```
   7.63413381305000       6.79703331400359          86.4579672009308       6.79703331400359
   7.94857831287022       6.99656103582411          74.9011771224587       6.99656103582411
   8.15445239797345       7.19761094044765          62.6153346249622       7.19761094044765
   8.25097207821786       7.39707777495605          49.8684485871005       7.39707777495605
   8.25302057582710       7.59660549677657          36.6395278100514       7.59660549677657
   8.14986224432484       7.79765540140011          22.9045732033600       7.79765540140011
   7.92321233875917       7.99712223590850          8.95386849082134       7.99712223590850
   7.57395601148037       8.19664995772902         -5.24617308620627       8.19664995772902
   7.10366125082743       8.39617767954954         -19.6138272767991       8.39617767954954
   6.51451564913777       8.59722758417308         -34.1820271345174       8.59722758417308
   6.00016552749258       8.79669441868148         -48.6477618340314       8.79669441868148
   5.96728839317947       8.99622214050199         -63.0524260190830       8.99622214050199
   5.86038712670840       9.19568897501039         -77.3097684766058       9.19568897501039
   5.68549341644331       9.39673887963393         -91.4570747011426       9.39673887963393
   5.44914475603662       9.59626660145445         -105.197738982054       9.59626660145445
   5.15856146937568       9.79579432327496         -118.562302984862       9.79579432327496
   4.82163406832737       9.99684422789851         -131.569809516722       9.99684422789851
#    50                                         #    50
#   0.33333                                     #   0.33333
! KI vs. Depth       (angle =   3.14159 radians)    ! Stress vs. Depth   (angle =   3.14159 radians)
  -9.37330239135706      0.199527721820517        -415.865139046354      0.199527721820517
  -13.0818120880370      0.400577626444059        -362.417859942598      0.400577626444059
  -15.8090696828671      0.600044460952455        -312.598530432091      0.600044460952455
  -18.0093821286639      0.799572182772972        -265.882196480447      0.799572182772972
  -19.8618778762487      0.999039017281368        -222.219909894520      0.999039017281368
  -21.4596608198313       1.20008892190491        -181.208123309176       1.20008892190491
  -22.9181454629560       1.39961664372543        -143.403634460936       1.39961664372543
  -24.2397630860521       1.59914436554594        -108.407220280277       1.59914436554594
  -25.1788109641668       1.79861120005434        -76.1508072269442       1.79861120005434
  -23.7833966921739       1.99966110467788        -46.3212892555369       1.99966110467788
  -22.2023467023383       2.19918882649840        -19.3026093727623       2.19918882649840
  -20.4799961910560       2.39865566100679         5.21149806455505       2.39865566100679
  -18.7509238830322       2.59970556563034         27.4730028680317       2.59970556563034
  -17.0434471156446       2.79923328745085         47.2149583515208       2.79923328745085
  -15.2851993904083       2.99876100927137         64.6925520590975       2.99876100927137
  -13.4984627352549       3.19822784377977         79.9789546729440       3.19822784377977
  -11.7033596110372       3.39927774840331         93.2536466248544       3.39927774840331
  -9.91753826750540       3.59880547022383         104.388626738665       3.59880547022383
  -8.17809724990545       3.79827230473222         113.567345471831       3.79827230473222
  -6.53565018170979       3.99780002655274         120.872897805888       3.99780002655274
  -4.93506411052133       4.19884993117628         126.414995598165       4.19884993117628
  -3.38739423060864       4.39837765299680         130.187723132565       4.39837765299680
  -1.90263741087899       4.59784448750519         132.316905751384       4.59784448750519
```

-0.489713607855721	4.79737220932571	132.881334690056	4.79737220932571
0.843266702975578	4.99842211394925	131.945057014631	4.99842211394925
2.08599916574867	5.19788894845765	129.601177488104	5.19788894845765
3.24064476099429	5.39741667027817	125.924244218561	5.39741667027817
4.30114244038550	5.59846657490171	120.950022439792	5.59846657490171
5.26208617211103	5.79799429672223	114.831838100921	5.79799429672223
6.11878500737469	5.99746113123062	107.616591169171	5.99746113123062
6.86712006405272	6.19698885305114	99.3773681000294	6.19698885305114
7.56086563277876	6.39803875767468	90.1202266159308	6.39803875767468
8.15723110901638	6.59750559218308	80.0665392741686	6.59750559218308
8.63427772410001	6.79703331400359	69.2210747009308	6.79703331400359
8.98991743474044	6.99656103582411	57.6642846224587	6.99656103582411
9.22276297694690	7.19761094044765	45.3784421249622	7.19761094044765
9.33192765043572	7.39707777495605	32.6315560871005	7.39707777495605
9.33424452065420	7.59660549677657	19.4026353100514	7.59660549677657
9.21757146964969	7.79765540140011	5.66768070336004	7.79765540140011
8.96122827751835	7.99712223590850	-8.28302400917867	7.99712223590850
8.56621605996075	8.19664995772902	-22.4830655862063	8.19664995772902
8.03430822665486	8.39617767954954	-36.8507197767991	8.39617767954954
7.36797896527553	8.59722758417308	-51.4189196345174	8.59722758417308
6.78624410098517	8.79669441868148	-65.8846543340314	8.79669441868148
6.74905975035895	8.99622214050199	-80.2893185190830	8.99622214050199
6.62815340441680	9.19568897501039	-94.5466609766058	9.19568897501039
6.43034695988661	9.39673887963393	-108.693967201143	9.39673887963393
6.16303438407325	9.59626660145445	-122.434631482054	9.59626660145445
5.83438193175135	9.79579432327496	-135.799195484862	9.79579432327496
5.45331384665473	9.99684422789851	-148.806702016722	9.99684422789851

Listing of Output Stress and Stress Intensity Files (WDdata25c15to17.fil and Wddata25c18to20.fil) for (25mm) Outer Lid Test Case

```
! Output from sccd version 1.01
! For sampled random variable z =  0.00000
! Stress vs. Depth
! argument in( 1) =      0.00000
! argument in( 2) =      1.00000
! argument in( 3) =   -356.26778
! argument in( 4) =     37.18077
! argument in( 5) =      1.43639
! argument in( 6) =     -0.06528
! argument in( 7) =      3.00000
! argument in( 8) =    322.12305
```

```
! Output from sccd version 1.01
! For sampled random variable z =  0.00000
! Stress Intensity vs. Depth
! argument in( 1) =      0.00000
! argument in( 2) =      1.00000
! argument in( 3) =   -356.26778
! argument in( 4) =     37.18077
! argument in( 5) =      1.43639
! argument in( 6) =     -0.06528
! argument in( 7) =      3.00000
! argument in( 8) =    322.12305
```

```
! argument in( 9) =      0.05000
! argument in(10) =     17.23689
! argument in(11) =      2.00000
! argument in(12) =     34.00000
! argument in(13) =     33.00000
#     3    2
#    50
#   0.33333
! Stress vs. Depth   (angle =   0.00000 radians)
  -341.215784707651       0.398800000000000
  -325.633364692085       0.800100000000000
  -309.739642115624        1.19890000000000
  -293.360529728595        1.60020000000000
  -276.725076327183        1.99900000000000
  -259.649895127803        2.40030000000000
  -242.372707600602        2.79910000000000
  -224.702081147980        3.20040000000000
  -206.883156194151        3.59920000000000
  -188.831551544850        3.99800000000000
  -170.457042366105        4.39930000000000
  -152.013539113604        4.79810000000000
  -133.294986374736        5.19940000000000
  -114.559581218197        5.59820000000000
  -95.5976084783162        5.99950000000000
  -76.6702981169005        6.39830000000000
  -57.6894435466940        6.79700000000000
  -38.5463100679875        7.19840000000000
  -19.5233934171268        7.59710000000000
 -0.388237329730828        7.99850000000000
   18.5767697770207        8.39720000000000
   37.6032998395972        8.79860000000000
   56.4104257774758        9.19730000000000
   75.2276811817238        9.59870000000000
   93.7769543259661        9.99740000000000
   112.165003299998        10.3962000000000
   130.475735164219        10.7975000000000
   148.456034096812        11.1963000000000
   166.306148033961        11.5976000000000
   183.778700225955        11.9964000000000
   201.067572676921        12.3977000000000
   217.932381429153        12.7965000000000
   234.559388834825        13.1978000000000
   250.716457448134        13.5966000000000
```

```
! argument in( 9) =      0.05000
! argument in(10) =     17.23689
! argument in(11) =      2.00000
! argument in(12) =     34.00000
! argument in(13) =     33.00000
#     3    2
#    50
#   0.33333
! KI vs. Depth       (angle =   0.00000 radians)
  -8.09691255300000       0.398800000000000
  -11.0886444800000       0.800100000000000
  -13.1274377800000        1.19890000000000
  -14.6239520700000        1.60020000000000
  -15.7412556300000        1.99900000000000
  -16.5649483400000        2.40030000000000
  -17.1663451100000        2.79910000000000
  -17.5702798000000        3.20040000000000
  -17.7952129600000        3.59920000000000
  -17.8596051600000        3.99800000000000
  -17.7778512400000        4.39930000000000
  -17.5614890600000        4.79810000000000
  -17.2275506700000        5.19940000000000
  -16.7851564800000        5.59820000000000
  -16.2344163700000        5.99950000000000
  -15.5815937400000        6.39830000000000
  -14.8325124700000        6.79700000000000
  -13.9923371100000        7.19840000000000
  -13.0624961600000        7.59710000000000
  -12.0377151800000        7.99850000000000
  -10.9313780700000        8.39720000000000
  -9.74728683200000        8.79860000000000
  -8.48932037700000        9.19730000000000
  -7.16114884300000        9.59870000000000
  -5.76640940000000        9.99740000000000
  -4.32730966500000        10.3962000000000
  -2.83079538300000        10.7975000000000
  -1.28043779400000        11.1963000000000
  0.320255595000000        11.5976000000000
   1.96775310200000        11.9964000000000
   3.65854282600000        12.3977000000000
   5.41509830400000        12.7965000000000
   7.21878315800000        13.1978000000000
   9.05768593000000        13.5966000000000
```

```
   266.483419038827        13.9954000000000
   281.930308024625        14.3967000000000
   296.839690652968        14.7955000000000
   311.373312900355        15.1968000000000
   325.325119867184        15.5956000000000
   338.844851817049        15.9969000000000
   351.739086423205        16.3957000000000
   364.068844440398        16.7945000000000
   375.880970062756        17.1958000000000
   387.003316895848        17.5946000000000
   397.550150527566        17.9959000000000
   407.365089477394        18.3947000000000
   416.546007559362        18.7960000000000
   424.953541926765        19.1948000000000
   432.667920899871        19.5961000000000
   439.568053985687        19.9949000000000
#    50
#   0.33333
! Stress vs. Depth   (angle =   1.57080 radians)
  -358.452677207651       0.398800000000000
  -342.870257192085       0.800100000000000
  -326.976534615624        1.19890000000000
  -310.597422228595        1.60020000000000
  -293.961968827183        1.99900000000000
  -276.886787627803        2.40030000000000
  -259.609600100602        2.79910000000000
  -241.938973647980        3.20040000000000
  -224.120048694151        3.59920000000000
  -206.068444044850        3.99800000000000
  -187.693934866105        4.39930000000000
  -169.250431613604        4.79810000000000
  -150.531878874736        5.19940000000000
  -131.796473718197        5.59820000000000
  -112.834500978316        5.99950000000000
  -93.9071906169005        6.39830000000000
  -74.9263360466939        6.79700000000000
  -55.7832025679875        7.19840000000000
  -36.7602859171268        7.59710000000000
  -17.6251298297308        7.99850000000000
   1.33987727702068        8.39720000000000
   20.3664073395972        8.79860000000000
   39.1735332774758        9.19730000000000
   57.9907886817238        9.59870000000000
```

```
   10.9282573600000        13.9954000000000
   12.8269042200000        14.3967000000000
   14.7498794700000        14.7955000000000
   16.7317527100000        15.1968000000000
   18.7698867000000        15.5956000000000
   20.8228550800000        15.9969000000000
   22.8864822400000        16.3957000000000
   24.9569222200000        16.7945000000000
   27.0302191900000        17.1958000000000
   29.1346134200000        17.5946000000000
   31.3332883800000        17.9959000000000
   33.5255900500000        18.3947000000000
   35.7070131700000        18.7960000000000
   37.8729426100000        19.1948000000000
   40.0186533300000        19.5961000000000
   42.1395302100000        19.9949000000000
#    50
#   0.33333
! KI vs. Depth       (angle =   1.57080 radians)
  -7.77940628749121       0.398800000000000
  -10.6538226790538       0.800100000000000
  -12.6126682653308        1.19890000000000
  -14.0504993646222        1.60020000000000
  -15.1239898195092        1.99900000000000
  -15.9153828603987        2.40030000000000
  -16.4931969078138        2.79910000000000
  -16.8812920053652        3.20040000000000
  -17.0974048048693        3.59920000000000
  -17.1592719773584        3.99800000000000
  -17.0807238943562        4.39930000000000
  -16.8728459788606        4.79810000000000
  -16.5520023988175        5.19940000000000
  -16.1269559232988        5.59820000000000
  -15.5978121235526        5.99950000000000
  -14.9705887913014        6.39830000000000
  -14.2508814332763        6.79700000000000
  -13.4436520806810        7.19840000000000
  -12.5502732173862        7.59710000000000
  -11.5656772313323        7.99850000000000
  -10.5027231962871        8.39720000000000
  -9.36506402539149        8.79860000000000
  -8.15642652493410        9.19730000000000
  -6.88033691487178        9.59870000000000
```

```
   76.5400618259661       9.99740000000000
   94.9281107999982       10.3962000000000
   113.238842664219       10.7975000000000
   131.219141596812       11.1963000000000
   149.069255533961       11.5976000000000
   166.541807725955       11.9964000000000
   183.830680176921       12.3977000000000
   200.695488929153       12.7965000000000
   217.322496334825       13.1978000000000
   233.479564948134       13.5966000000000
   249.246526538827       13.9954000000000
   264.693415524625       14.3967000000000
   279.602798152968       14.7955000000000
   294.136420400355       15.1968000000000
   308.088227367184       15.5956000000000
   321.607959317049       15.9969000000000
   334.502193923205       16.3957000000000
   346.831951940398       16.7945000000000
   358.644077562756       17.1958000000000
   369.766424395848       17.5946000000000
   380.313258027566       17.9959000000000
   390.128196977394       18.3947000000000
   399.309115059362       18.7960000000000
   407.716649426765       19.1948000000000
   415.431028399871       19.5961000000000
   422.331161485687       19.9949000000000
#    50
#   0.33333
! Stress vs. Depth   (angle =   3.14159 radians)
  -375.689569707651      0.398800000000000
  -360.107149692085      0.800100000000000
  -344.213427115624       1.19890000000000
  -327.834314728595       1.60020000000000
  -311.198861327183       1.99900000000000
  -294.123680127803       2.40030000000000
  -276.846492600602       2.79910000000000
  -259.175866147980       3.20040000000000
  -241.356941194151       3.59920000000000
  -223.305336544850       3.99800000000000
  -204.930827366105       4.39930000000000
  -186.487324113604       4.79810000000000
  -167.768771374736       5.19940000000000
  -149.033366218197       5.59820000000000
```

```
  -5.54028973994384       9.99740000000000
  -4.15762178428735       10.3962000000000
  -2.71979069268223       10.7975000000000
  -1.23022766519743       11.1963000000000
  0.307697331919948       11.5976000000000
   1.89059110540318       11.9964000000000
   3.51507946730819       12.3977000000000
   5.20275469418431       12.7965000000000
   6.93571120100262       13.1978000000000
   8.70250461675730       13.5966000000000
   10.4997248594721       13.9954000000000
   12.3239196032991       14.3967000000000
   14.1714887418589       14.7955000000000
   16.0756462887444       15.1968000000000
   18.0338584187100       15.5956000000000
   20.0063232340148       15.9969000000000
   21.9890288639026       16.3957000000000
   23.9782801609685       16.7945000000000
   25.9702764161681       17.1958000000000
   27.9921505067011       17.5946000000000
   30.1046082732897       17.9959000000000
   32.2109426672998       18.3947000000000
   34.3068250946231       18.7960000000000
   36.3878213995116       19.1948000000000
   38.4493918261455       19.5961000000000
   40.4871022283844       19.9949000000000
#    50
#   0.33333
! KI vs. Depth       (angle =   3.14159 radians)
  -7.46190002198242      0.398800000000000
  -10.2190008781076      0.800100000000000
  -12.0978987506616       1.19890000000000
  -13.4770466592444       1.60020000000000
  -14.5067240090184       1.99900000000000
  -15.2658173807974       2.40030000000000
  -15.8200487056275       2.79910000000000
  -16.1923042107303       3.20040000000000
  -16.3995966497387       3.59920000000000
  -16.4589387947168       3.99800000000000
  -16.3835965487123       4.39930000000000
  -16.1842028977212       4.79810000000000
  -15.8764541276350       5.19940000000000
  -15.4687553665976       5.59820000000000
```

-130.071393478316	5.99950000000000	-14.9612078771051	5.99950000000000
-111.144083116901	6.39830000000000	-14.3595838426029	6.39830000000000
-92.1632285466939	6.79700000000000	-13.6692503965527	6.79700000000000
-73.0200950679875	7.19840000000000	-12.8949670513620	7.19840000000000
-53.9971784171268	7.59710000000000	-12.0380502747723	7.59710000000000
-34.8620223297308	7.99850000000000	-11.0936392826645	7.99850000000000
-15.8970152229793	8.39720000000000	-10.0740683225743	8.39720000000000
3.12951483959724	8.79860000000000	-8.98284121878298	8.79860000000000
21.9366407774758	9.19730000000000	-7.82353267286819	9.19730000000000
40.7538961817238	9.59870000000000	-6.59952498674356	9.59870000000000
59.3031693259661	9.99740000000000	-5.31417007988769	9.99740000000000
77.6912182999982	10.3962000000000	-3.98793390357469	10.3962000000000
96.0019501642188	10.7975000000000	-2.60878600236445	10.7975000000000
113.982249096812	11.1963000000000	-1.18001753639487	11.1963000000000
131.832363033961	11.5976000000000	0.295139068839897	11.5976000000000
149.304915225955	11.9964000000000	1.81342910880635	11.9964000000000
166.593787676921	12.3977000000000	3.37161610861639	12.3977000000000
183.458596429153	12.7965000000000	4.99041108436861	12.7965000000000
200.085603834825	13.1978000000000	6.65263924400525	13.1978000000000
216.242672448134	13.5966000000000	8.34732330351461	13.5966000000000
232.009634038827	13.9954000000000	10.0711923589443	13.9954000000000
247.456523024625	14.3967000000000	11.8209349865983	14.3967000000000
262.365905652968	14.7955000000000	13.5930980137178	14.7955000000000
276.899527900355	15.1968000000000	15.4195398674887	15.1968000000000
290.851334867184	15.5956000000000	17.2978301374200	15.5956000000000
304.371066817049	15.9969000000000	19.1897913880297	15.9969000000000
317.265301423205	16.3957000000000	21.0915754878051	16.3957000000000
329.595059440398	16.7945000000000	22.9996381019371	16.7945000000000
341.407185062756	17.1958000000000	24.9103336423363	17.1958000000000
352.529531895848	17.5946000000000	26.8496875934023	17.5946000000000
363.076365527566	17.9959000000000	28.8759281665795	17.9959000000000
372.891304477394	18.3947000000000	30.8962952845995	18.3947000000000
382.072222559362	18.7960000000000	32.9066370192463	18.7960000000000
390.479756926765	19.1948000000000	34.9027001890233	19.1948000000000
398.194135899871	19.5961000000000	36.8801303222910	19.5961000000000
405.094268985687	19.9949000000000	38.8346742467688	19.9949000000000

All other test files are available for review and documented in DTN: MO0002SPASDA04.001.

4. REFERENCES

CRWMS M&O 1999f. *Testing of Software Routine to Determine Deviate and Cumulative Probability: ModStandardNormal Version 1.0.* CAL-EBS-MD-000004 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991018.0213.

CRWMS M&O 2000h. *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier and the Stainless Steel Structural Material.* ANL-EBS-MD-000005 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0259

Golder Associates 2000. *User's Guide, GoldSim, Graphical Simulation Environment.* Version 6.02. Manual Draft #4 (March 17, 2000). Redmond, Washington: Systems Simulation Group Golder Associates Inc. TIC: 247347.

MO0004SPASDA04.003. Revised Supporting Data for Abstraction of Models for Stress Corrosion Cracking of WP Outer Barrier Closure Lid Welds. Submittal date: 02/03/2000. Submit to RPC URN-0266

ATTACHMENT IV

PREWAP SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Software Name and Version Number: PREWAP Version 1.0

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 6.0A, Professional Edition.

SRR Document Identification Number: N/A

SRR Media Number (If Applicable): N/A

2. DESCRIPTION AND TESTING

2.1 OVERVIEW

Corrosion of the drip shields and waste packages is accounted for in the Total System Performance Assessment-Site Recommendation (TSPA-SR) model by the WAPDEG routine, which runs as a DLL under the TSPA-SR software (Golder Associates 2000). As input, WAPDEG requires T-H data (temperatures, relative humidities, etc.), as well as seepage chemistry information (pH, chloride concentration, etc.). T-H data are taken from CRWMS M&O 2000k. Seepage chemistry in-drift is characterized in the AMR entitled *In-Drift Precipitates/Salts Analysis* (CRWMS M&O 2000l). In-package chemistry is characterized in the AMR entitled *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m).

The PREWAP routine calculates the seepage chemistry associated with the T-H data. The T-H and seepage chemistry data are then written to output files that are used as input to the WAPDEG routine (CRWMS M&O 1999e).

The PREWAP routine extracts this data from these various tables and prepares an output table that is used as input to the WAPDEG routine.

The PREWAP routine is a stand-alone executable that does not operate as a DLL under TSPA-SR software (i.e., Goldsim (Golder Associates 2000)). This allows the WAPDEG input to be prepared independent of (TSPA-SR) software, reducing the run time for TSPA-SR realizations.

2.2 INPUTS

The input to PREWAP consist of in-drift drip and no-drip chemistry pH and Cl data, in-package pH and Cl data, and T-H data (for low, mean, and high infiltration cases) (CRWMS M&O 2000k) for Commercial Spent Nuclear Fuel (CSNF) and Co-Disposed Waste Package (CDSP) waste packages. Information is also passed to PREWAP regarding input and output file names, as well as an RH corrosion limit.

2.2.1 In-Drift Chemistry Data (Drip Conditions)

In-drift pH and Chloride Concentration (Cl) under dripping conditions are dependent on RH and the abstracted time period. Within a given set of RH and time period, they can also be dependent on temperature (T), invert evaporation rate (Q_e), and seepage rate (Q_s) into the drift. The break-down of cases and their independent parameters are given in Table 1.

Table 1. Classification of In-Drift pH and Cl Data Sets for Dripping Conditions

	RH	time period(s)*	additional independent parameters
case 1	RH<50.3%	all	none
case 2	50.3%<RH<85%	2, 3, 4, 5	none
case 3	RH>85%	2, 3, 5	1-Qe/Qs
case 4	RH>85%	4	1-Qe/Qs, T

*time periods:
1 0 to 50 years from initial opening of the repository
2 50 to 1000 years from initial opening of the repository
3 1000 to 2000 years from initial opening of the repository
4 2000 to 100,000 years from initial opening of the repository
5 > 100,000 years from initial opening of the repository

Case 1 conditions have no pH and Cl (Molal) data. For this case, the pH and Cl are hardwired in the PREWAP code to be equal to -9.99E-02 (the default 'does not exist' value for WAPDEG input).

Case 2 data for pH and Cl are contained in files **phTable1.dat** and **ClTable1.dat**, respectively. The contents of these files are shown in Table 2 and Table 3. The value in the first row indicates the number of rows of data to follow. The data are organized as a set of 1-D look-up tables. The 1st column contains the RH independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for time periods 2, 3/5, and 4, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Case 3 data for pH and Cl are contained in files **phTable2.dat** and **ClTable2.dat**, respectively. The contents of these files are shown in Table 4 and Table 5. The value in the first row indicates the number of rows of data to follow. The data are organized as a set of 1-D look-up tables. The 1st column contains the 1-Q_e/Q_s independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for time periods 2 and 3/5, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Case 4 data for pH and Cl are contained in files **phTable3.dat** and **ClTable3.dat**, respectively. The contents of these files are shown in Table 6 and Table 7. The values in the first row indicate the number of rows and columns that make up the dependent data set (pH or Cl values) in the 2-

D look-up table that follows. The next row contains the independent parameter temperature values. In the remaining rows, the 1st column contains the 1-Q_e/Q_s independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for temperatures of 25 C, 50 C, and 75 C, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Table 2. Case 2 pH Look-Up Table (In-Drift Dripping Conditions)

10			
50.3	9.40	7.64	7.02
51.0	9.40	7.64	7.02
53.1	9.40	7.64	7.02
55.2	9.40	7.64	7.02
60.5	9.40	7.64	7.02
65.7	9.40	7.64	7.02
71.0	9.40	7.64	7.02
76.2	9.40	7.64	7.02
81.5	9.40	7.64	7.02
85.0	9.40	7.64	7.02
	2	3/5 4	

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = pH

Table 3 Case 2 Cl Look-Up Table (In-Drift Dripping Conditions)

10			
50.3	-2.431	-2.428	-2.415
51.0	-1.246	-1.244	-1.231
53.1	-0.389	-0.391	-0.380
55.2	-0.164	-0.169	-0.159
60.5	0.225	0.211	0.216
65.7	0.380	0.358	0.359
71.0	0.420	0.396	0.396
76.2	0.428	0.403	0.403
81.5	0.418	0.394	0.394
85.0	0.407	0.382	0.382
	2	3/5	4

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))

Table 4. Case 3 pH Look-Up Table (In-Drift Dripping Conditions)

7		
0.000999	9.40	7.64
0.001	9.41	7.64
0.01	9.28	7.58
0.1	9.21	7.45
0.5	8.87	7.64
0.9	8.62	7.71
1.0	8.58	7.72
	2	3/5

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = 1-Qe/Qs (Qe = evaporation rate, Qs = incoming seepage rate)
; condition: relative humidity (RH) > 85 percent
; dependent parameter = pH

Table 5. Case 3 Cl Look-Up Table (In-Drift Dripping Conditions)

7		
0.000999	0.387	0.382
0.001	0.190	0.373
0.01	-0.752	-0.502
0.1	-1.745	-1.496
0.5	-2.445	-2.194
0.9	-2.699	-2.449
1.0	-2.745	-2.496
	2	3/5

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = 1-Qe/Qs (Qe = evaporation rate, Qs = incoming seepage rate)
; condition: relative humidity (RH) > 85 percent
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))

Table 6. Case 4 pH Look-Up Table (In-Drift Dripping Conditions)

7	3		
25		50	75
0.0011999	7.02	7.02	7.02
0.0012	6.78	6.86	7.02
0.01	6.986	6.95	7.02
0.1	7.11	7.03	6.97
0.5	7.23	7.18	7.14
0.9	7.09	7.22	7.18
1.0	7.05	7.22	7.19

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; condition: Period 4
; 1st independent variable (columns) = temperature ('C)
; dependent parameter = pH

Table 7. Case 4 Cl Look-Up Table (In-Drift Dripping Conditions)

7	3		
25		50	75
0.0011999	0.38202	0.38202	0.38202
0.0012	0.39094	0.38202	0.38202
0.01	-0.48798	-0.48872	-0.48945
0.1	-1.4828	-1.48216	-1.48214
0.5	-2.18053	-2.18052	-2.18059
0.9	-2.43581	-2.43581	-2.43581
1.0	-2.48149	-2.48149	-2.48162

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water

```
; dependent parameter = log Cl (i.e., log of Cl concentration (Molal))
```

2.2.2 In-Drift Chemistry Data (No-Drip Conditions)

In-drift pH under no-dripping conditions is dependent on CO2 fugacity and temperature. No-drip pH data are contained in file **phTable4.dat**a. The contents of this file are shown in Table 8. The values in the first row indicate the number of rows and columns that make up the dependent data set (pH values) in the 2-D look-up table that follows. The next row contains the independent parameter temperature values. In the remaining rows, the 1st column contains the independent parameter log CO2 fugacity values. Columns 2, 3, 4, and 5 contain the dependent parameter values (pH) for temperatures of 25 C, 45 C, 75 C, and 95 C, respectively. The remaining information in the file below the look-up table (column headings) is not used by PREWAP.

There are no data for Cl under no-dripping conditions; hence the no-drip Cl is hardwired in the PREWAP code to be equal to the default 'does not exist' value of -9.99E-02.

Table 8. pH Look-Up Table (In-Drift No-Dripping Conditions)

7		4		
25		45	75	95
-1	4.41	4.47	4.60	4.70
-3	5.41	5.49	5.73	6.02
-4	5.91	6.03	6.41	6.70
-5	6.39	6.57	6.88	6.96
-6	6.80	6.92	6.99	7.00
-7	6.97	6.99	7.00	7.00
-9	7.00	7.00	7.00	7.00
log fCO2				

2.2.3 In-Package Chemistry Data (Drip and No-Drip Conditions)

In-Package chemistry is dependent upon the waste type (CSNF or CDSP) in the waste package. Bounding values for the pH and Cl are read into PREWAP from the file **InPkgChem.dat**. The 1st row contains the bounding pH values for CSNF and CDSP, respectively. The 2nd row contains the bounding Cl value used for both CSNF and CDSP.

Table 9. pH and Cl In-Package Chemistry Data

7.60	9.83
2.014E-04	

For CSNF, the in-package chemistry is a function of cladding coverage and seepage flow rate. Inspection of Figures 4.3 and 4.4 in the *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m) finds that the >1000 year post-breach period has the potential to have the highest pH within the bounds of the response surface data-set. Using the appropriate equation from Table 4.6 (CRWMS M&O 2000m) yields the upper bound on pH for CSNF.

$$pH = 6.0668 - 0.5395\log(cc) + 4.0479\left[\frac{yr}{mm}\right]Q$$

$$pH = 6.0668 - 0.5395\log(0.02) + 4.0479\left[\frac{yr}{mm}\right]\left(0.15\frac{mm}{yr}\right) = 7.60$$

The terms *cc* and *Q* represent cladding coverage fraction and flow rate (mm/yr), respectively. For CDSP the in-package chemistry is a function of relative glass rate and seepage flow rate. The glass rate is a relative dissolution rate and is described in further detail in the *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m). Inspection of Figures 4.5 and 4.6 in the *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m) finds that the >1000 year post-breach period has the potential to have the highest pH within the bounds of the response surface data-set. Using the appropriate equation from Table 4.11 (CRWMS M&O 2000m) yields the upper bound on pH for CSNF.

$$pH = 8.4247 - 3.4173\left[\frac{yr}{mm}\right]Q + 0.1403GR$$

$$pH = 8.4247 - 3.4173\left[\frac{yr}{mm}\right]\left(0.0015\frac{mm}{yr}\right) + 0.1403(10.0) = 9.83$$

The terms Q and GR represent the seepage and glass rate, respectively. A chloride value of 2.014E-04 mol/kg (equal to that of J-13 water) is specified for both CSNF and CDSP waste package (CRWMS M&O 2000m).

2.2.4 T-H Data

The T-H data sets are broken down into five ‘bins’ based on infiltration rate. Furthermore, there are separate sets of T-H data for each infiltration scenario (low, mean, or high). Table 10 shows the relationship between infiltration bins, infiltration scenario, and the T-H data files.

Table 10 Relationship Between Infiltration Bins, Infiltration Scenario, and T-H Data Files

	infiltration scenario		
infiltration bin	**low**	**mean**	**high**
bin 1 (< 3.4 mm/yr)	CSNF_low_Bin1.in HLW_low_Bin1.in	CSNF_mean_Bin1.in HLW_mean_Bin1.in	n/a n/a
bin 2 (3.4 to 10 mm/yr)	CSNF_low_Bin2.in HLW_low_Bin2.in	CSNF_mean_Bin2.in HLW_mean_Bin2.in	CSNF_high_Bin2.in HLW_high_Bin2.in
bin 3 (10 to 20 mm/yr)	n/a n/a	CSNF_mean_Bin3.in HLW_mean_Bin3.in	CSNF_high_Bin3.in HLW_high_Bin3.in
bin 4 (20 to 60 mm/yr)	n/a n/a	CSNF_mean_Bin4.in HLW_mean_Bin4.in	CSNF_high_Bin4.in HLW_high_Bin4.in
bin 5 (> 60 mm/yr)	n/a n/a	CSNF_mean_Bin5.in HLW_mean_Bin5.in	CSNF_high_Bin5.in HLW_high_Bin5.in

The format of the T-H files is illustrated in Table 11.

Table 11 T-H File CSNF_mean_Bin5.in

line(s)	T-H file information	comment
1	Infiltration Bin:	not used
2	qinf > 60.0 mm/yr	not used
3	RIP_csnf_d0010500_bin-60_mean	not used
4	data column headers (see below)	not used
5	The number of Rows = 83	numeric value read in
6	The fraction of this history = 0.000576	numeric value read in
7	Coordinate Location:	not used
8	The easting coordinate = 170208.78 m	not used
9	The northing coordinate = 234316.70 m	not used
10	Infiltration rate:	not used
11	qinf = 61.00266 mm/yr	not used
12 to 94	T-H data	read in
95	The number of Rows = 84	numeric value read in
96	The fraction of this history = 0.000960	numeric value read in
97	Coordinate Location:	not used
98	The easting coordinate = 170228.75 m	not used
99	The northing coordinate = 234315.60 m	not used
100	Infiltration rate:	not used
101	qinf = 60.79187 mm/yr	not used
102 to 195	T-H data	read in
196	The number of Rows = 87	numeric value read in
197	The fraction of this history = 0.001153	numeric value read in
198	Coordinate Location:	not used
199	The easting coordinate = 170256.20 m	not used
200	The northing coordinate = 234314.20 m	not used
201	Infiltration rate:	not used
202	qinf = 60.37322 mm/yr	not used
203 to 290	T-H data	read in

Each T-H data file contains time-histories from zero to one-million years for the following parameters at a given number of spatial locations:

Waste Package Temperature [C]
Drip Shield Temperature [C]
Drift Wall Temperature [C]
Invert Temperature [C]
Waste Package RH [-]
Drip Shield RH [-]
Drift Wall RH [-]

Backfill RH [-]
Invert RH [-]
Liquid Saturation at the Drip Shield [-]
Liquid Saturation at the Invert [-]
Air Mass Fraction [-]
Water Vapor Flux at Drift Wall [kg/yr/m of drift]
Air Flux at Drift Wall [kg/yr/m of drift]
Drip Shield Water Evaporation Rate [m3/yr]
Backfill Water Evaporation Rate [m3/yr]
Invert Water Evaporation Rate [m3/yr]
Percolation Flux at 5 m [mm/yr]
Volume flow at the Drip Shield Top [m3/yr]
Volume flow at the Invert [m3/yr]
Top of the Drip Shield Temperature [C]

2.2.5 Input/Output Control Files

The **InMaster.in** and **OutMaster.in** files pass file-name information to PREWAP. The 1st row in **InMaster.in** contains the number of file names. The remaining rows list the names of the T-H files that are to be read by PREWAP. **OutMaster.in** contains the names of the WAPDEG input files that PREWAP results are to be written.

Table 12 InMaster.in File

```
22
CSNF_low_bin1.in
CSNF_low_bin2.in
HLW_low_bin1.in
HLW_low_bin2.in
CSNF_mean_bin1.in
CSNF_mean_bin2.in
CSNF_mean_bin3.in
CSNF_mean_bin4.in
CSNF_mean_bin5.in
HLW_mean_bin1.in
HLW_mean_bin2.in
HLW_mean_bin3.in
HLW_mean_bin4.in
HLW_mean_bin5.in
CSNF_high_bin2.in
CSNF_high_bin3.in
CSNF_high_bin4.in
CSNF_high_bin5.in
HLW_high_bin2.in
HLW_high_bin3.in
HLW_high_bin4.in
HLW_high_bin5.in
```

Table 13 OutMaster.in File

```
CSNF_low_bin1.ou
CSNF_low_bin2.ou
HLW_low_bin1.ou
HLW_low_bin2.ou
CSNF_mean_bin1.ou
CSNF_mean_bin2.ou
CSNF_mean_bin3.ou
CSNF_mean_bin4.ou
CSNF_mean_bin5.ou
HLW_mean_bin1.ou
HLW_mean_bin2.ou
HLW_mean_bin3.ou
HLW_mean_bin4.ou
HLW_mean_bin5.ou
CSNF_high_bin2.ou
CSNF_high_bin3.ou
CSNF_high_bin4.ou
CSNF_high_bin5.ou
HLW_high_bin2.ou
HLW_high_bin3.ou
HLW_high_bin4.ou
HLW_high_bin5.ou
```

2.3 DESCRIPTION OF SOFTWARE ROUTINE INCLUDING THE EXECUTION ENVIRONMENT

2.3.1 Development and Execution Environment

The PREWAP routine is a FORTRAN executable. The code was developed and tested in the Windows NT 4.0 operating system. It was compiled with Digital FORTRAN Professional 6.0A as a stand-alone executable (exe) program. The routine operates in a Windows 95/98 or Windows NT environment

2.3.2 Main Program

The PREWAP program begins by calling a subroutine (**ReadMasterFiles**) that reads in the T-H input and WAPDEG output file names. Next it calls a subroutine (**ReadChemData**) to read in the in-drift chemistry lookup tables and in-package chemistry data. The program then initiates a loop that calls subroutines that; read in the T-H data, perform the necessary calculations, and generate the WAPDEG input files.

The program loop first calls a subroutine to count the data sets(**CountDataSets**) in the selected T-H file. It then calls a subroutine to allocate arrays (**AllocateArays**) to hold the data during processing. Next a subroutine (**ReadInputFile**) reads the T-H data. The data are then processed by a subroutine (**DoCalculations**) that performs the necessary calculations. The next subroutine (**CullDataPoints**) checks the data set resulting from the calculations and eliminates (based on a threshold RH value) those portions that will not contribute to corrosion of the EBS. This modified dataset is in turn checked by the **AddDataPoints** subroutine to determine if minimum time-step size requirements are met. If they are not, interpolated data points are added back to the data set between the times that do not meet the minimum time-step requirements. The data set is then written to an output file by the **WriteOutputFile** subroutine. Finally it calls a subroutine (**DeallocateArrays**) to deallocate the arrays allocated earlier in the loop.

2.3.4 Subroutine ReadMasterFiles

The **ReadMasterFiles** subroutine opens the files **InMaster.in** and **OutMaster.in**. The RH corrosion limit and the number of T-H and WAPDEG input files are read in. A do-loop is then initiated that reads in the input file names (T-H files) from **InMaster.in** and the output file names (WAPDEG files) from **OutMaster.in**.

2.3.5 Subroutine ReadChemData

This subroutine reads in the Cl and pH look-up tables from files **CLtable1.dat**, **CLtable2.dat**, **Cltable3.dat**, **pHtable1.dat**, **pHtable2.dat**, **pHtable3.dat**, and **pHtable4.dat**. In-package chemistry data are read in from the file **InPkgChem.dat**. The data contained in these files are described Section 2.2.

2.3.6 Subroutine CountDataSets

This subroutine counts the number of data sets in each of the T-H files. It initializes the number of data sets (**nDataSets**) counter to 1 and the maximum number of rows (**maxRows**) variable to 0. The subroutine then reads past the 1st four rows of header information to the 5th row. It then reads past the header information in row 5 and reads the number of rows listed for that data set. This value is assigned to the variable **rows**. It then sets the value of **maxRows** equal to the number of rows just read.

The subroutine then reads past the next six rows of header information to the 1st data set. It then initiates a do-loop that executes **rows** number of times to read past the 1st data set.

It then begins to read the rest of the file with a do-loop. It reads the 1st header row for the next data set. If the end of file is reached the subroutine exits the do loop. If not, the subroutine reads the number of rows in the next data set as **rows**. It then increments the counter, **nDataSets**, by 1 and tests to see if the number of rows in this data set is greater than **maxrows**. If so, **maxrows** is set equal to **rows**. It then reads through this data set and restarts the loop. This loop is repeated until the end of file is reached. When the end of file is reached, the subroutine exits the do loop and closes the data file. The subroutine is then exited back to the main program.

2.3.7 Subroutine AllocateArays

This subroutine sets the bounds on dynamic arrays to match the maximum number of rows (**maxRows)** and number of data sets (**nDataSets**) counted in the subroutine **CountDataSets**.

2.3.8 Subroutine ReadInputFile

This subroutine reads the data from the T-H file to the dynamic arrays established in the previous subroutine.

2.3.9 Subroutine DoCalculations

This subroutine calculates pH and pH^2 for the waste package and the drip shield under drip and no drip conditions. Source Code is included for calculating Cl chemistry, but it is commented out. It also sets the in-package and barrier interface pH values for drip and no drip conditions.

The subroutine begins with a do-loop that sequentially processes each data set read from the TH file. Inside this loop is another do-loop that sequentially processes each row of data in the data set to calculate pH and pH^2 for the waste package and the drip shield. First it calculates the waste package pH and pH^2 for both drip and no drip conditions by calling the **InDriftCalc** subroutine using arguments that are specific to the waste package. Next it calculates the drip shield pH and pH^2 for both drip and no drip conditions by again calling the **InDriftCalc** subroutine, but using arguments that are specific to the drip shield.

After these calculations the subroutine sets the in-package pH for drip conditions for the waste package to the appropriate bounding value (pH of 7.6 for CSNF, 9.8 for Defense High Level Waste, and 9.83 for CDSP). It then sets the in-package pH for no-drip conditions equal to the default 'does not exist' value of -9.99E-02. Values for pH^2 are calculated from the pH values.

This process is repeated for each row of data in the data set. After all rows in a data set have been processed, the code processes the next data set until all data sets have been processed.

2.3.10 Subroutine InDriftCalc

The **InDriftCalc** subroutine is called by the **DoCalculations** subroutine. It performs the pH and pH^2 calculations for drip and no drip conditions for each row of data in the data set. The subroutine begins by first checking to see if the temperature is less than zero or if the seep rate is less than –99. If either condition applies, the pH for drip and no drip conditions is set to the default 'does not exist' value of -9.99E-02. If neither condition applies, the routine calculates 1-Q_e/Q_s for the row of data.

An **if-then-else** statement is used to determine which of the time periods is applicable. Values of drip and no-drip pH in the >50 year time period are set equal to the default 'does not exist' value of –9.99E-02. For the remaining time periods, an **if-then-else** statement is used to determine the applicable pH data-set based on RH. Table 14 shows the relationships between time periods, RH ranges, the potential independent parameters, and the pH data-sets.

Table 14 In-Drift Chemistry

time period	RH	drip condition	log(fCO2)	1-Q_e/Q_s	T	applicable point-value or data-set
>50 yrs	n/a	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
50 to 1000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	9.40
		no drip	**-6.5**		**T**	phTable4
	RH > 85	drip	n/a	**1-Q_e/Q_s**	n/a	phTable2a
		no drip	**-6.5**	n/a	**T**	phTable4
1000 to 2000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	7.64
		no drip	**-3.0**	n/a	**T**	phTable4
	RH > 85	drip	n/a	**1-Q_e/Q_s**	n/a	phTable2b
		no drip	**-3.0**	n/a	**T**	phTable4
2000 to 100,000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	7.02
		no drip	**-2.0**	n/a	**T**	phTable4
	RH > 85	drip	n/a	**1-Q_e/Q_s**	**T**	phTable3
		no drip	**-2.0**	n/a	**T**	phTable4
<100,000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip		n/a	n/a	7.64
		no drip	**-3.0**	n/a	**T**	phTable4
	RH > 85	drip		**1-Q_e/Q_s**	n/a	phTable2b
		no drip	**-3.0**	n/a	**T**	phTable4

As an example, the subroutine **Interp1D** is used to select pH values from the pH data-sets **phTable2a** and **phTable2b**, while subroutine **Interp2D** is used to select pH values from the pH data-sets **phTable3** and **phTable4**. In Table 14 the independent parameters associated with the pH data sets are denoted by **bold-face** type.

After these tests and calculations are performed to determine the values for pH under drip and no drip conditions, the values for pH^2 for drip and no drip conditions are calculated.

2.3.11 Subroutine Interp1D

This subroutine is called by the **InDriftCalc** subroutine to interpolate thermophysical properties such as pH values, from one-dimensional arrays (e.g. **phTable2a** and **phTable2b**) created when the in-drift chemistry data from and **phTable2.dat** file were read. The subroutine is passed the value of the independent variable, the independent and dependent variable vectors, and the number of rows in the passed vectors. The subroutine passes back the interpolated dependent variable value.

The subroutine first checks to see if the independent variable value is within the upper and lower bounds of the independent variable vector. If it is above the upper bound, the dependent variable value is set equal to its upper bound; if it is below the lower bound the dependent variable is set equal to its lower bound. If neither condition is met, the subroutine linearly interpolates the dependent variable value between the independent vector values bounding the independent variable.

2.3.12 Subroutine Interp2D

This subroutine is called by the **InDriftCalc** subroutine to interpolate thermophysical properties such as pH values from two dimensional arrays (e.g. **phTable3** and **phTable4**) created when the in-drift chemistry data from the **phTable3.dat** and **phTable4.dat** files were read. The subroutine is passed the values of the two independent variable, the two independent variable vectors, the dependent variable array, and the number of rows and columns passed array. The subroutine passes back the interpolated dependent variable value.

This subroutine first checks the value of the 1st independent variable to see if it is within the range of the 1st independent variable vector. If it is outside the range of the independent vector, a flag is set denoting whether it is above or below the range of the 1st independent vector. If the value of the 1st independent variable is within the range of the 1st independent vector, the subroutine loops through the 1st independent vector to identify the first row where the value of the 1st independent vector is less than the 1st independent variable.

Next the subroutine checks the value of the 2nd independent variable to see if it is within the range of the 2nd independent variable vector. If it is outside the range of the independent vector, a flag is set denoting whether it is above or below the range of the 2nd independent vector. If the value of the 2nd independent variable is within the range of the 2nd independent vector, the subroutine loops through the 2nd independent vector to identify the first row where the value of the 2nd independent vector is less than the 2nd independent variable.

The subroutine then checks to see if the 1st independent variable lower bound flag is set. If so, it then checks to see if the 2nd independent variable lower or upper bound flag is set. If this condition is satisfied, the dependent variable is assigned the value of the applicable corner point in the 2D array. If the 2nd independent variable is within the bounds of the 2nd independent vector, the subroutine linearly interpolates the dependent variable value between the 2nd independent vector values bounding the independent variable (i.e. along the lower edge of the array).

If the 1st independent variable is not outside the lower bound, the same process is repeated to determine if it is outside the upper bound. If this condition is satisfied, the dependent variable is set to the value at the upper corner points of the array or along the upper edge of the array.

The same logic is then repeated to identify values that are outside the upper and lower bounds of the 2nd independent variable.

If the 1st and 2nd independent variables are both within the bounds of their respective vectors, the program linearly interpolates the j-th column value between the i and i+1 rows. It then linearly interpolates the i-th row value between the j-th and j+1 columns. The results of these calculations are then used to linearly interpolate the dependent variable value.

2.3.13 Subroutine CullDataPoints

This subroutine removes rows of data where the waste package or drip shield temperature or RH are outside predetermined values. The subroutine loops through each data set. In turn each data-set is looped through (excepting the last row). A flag (**corFlag**) is set, based on a series of tests, to indicate whether or not that row of data is to be retained.

The **corFlag** is initialized to zero, as is the counter **nnRows()** which keeps track of the number of rows that are retained from each data-set.

The subroutine first checks to see if the waste package temperature or drip shield temperature is less than zero (values less than zero denote temperatures that 'do not exist'). If the condition is satisfied, the subroutine skips the remaining tests with **corFlag** set to zero. If the conditions are not satisfied, then the next test is performed with the **corFlag** variable still equal to zero.

Next the waste package and drip shield RH are checked to see if they are greater than the **corLim** value. If either is greater than **corLim**, **corFlag** is set to one and the remaining tests are skipped. Otherwise, **corFlag** remains at zero and the next test is performed.

Next the waste package RH for this row of data is checked to see if it is less than **corLim,** and the waste package RH for the next row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one and the remaining tests are skipped. Otherwise, **corFlag** remains at zero, and the next test is performed.

Next the drip shield RH for this row of data is checked to see if it is less than **corLim,** and the drip shield RH for the next row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, it remains at zero, and the next test is performed.

Next the waste package RH for this row of data is checked to see if it is less than **corLim,** and the waste package RH for the previous row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, **corFlag** remains at zero, and the next test is performed.

Next the drip shield RH for this row of data is checked to see if it is less than **corLim,** and the drip shield RH for the previous row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, **corFlag** remains at zero and the next test is performed.

Next the waste package RH for the current row of data, the preceding row of data, and the next row of data are checked to see if they are all less than **corLim**. If these conditions are met, the remaining tests are skipped, with **corFlag** remaining at zero. If these conditions are not met, the next test is performed.

Next the drip shield RH for the current row of data, the preceding row of data, and the next row of data, are checked to see if they are all less than **corLim**. If these conditions are met, the final test is skipped, with **corFlag** remaining at zero. If these conditions are not met, **corFlag** is set to one.

If **corFlag** is set to one by any of the preceding tests, the row of data is written to a temporary file (**temp.dat**) and **nnRows()** is incremented by one.

The last row of data is written to the temporary file for all of the data sets.

When all of the data-sets have been processed, the temporary file is closed.

2.3.14 Subroutine AddDataPoints

This subroutine steps through the time histories in the temporary file (**temp.dat**) created by the **CullDataPoints** subroutine and determines if time-step sizes above 50,000 years are sufficiently small. This is accomplished in two parts. For time periods from 50,000 to 200,000 years, the time-step interval should be no greater than 10,000 years. For time periods greater than 200,000 years, the time-step interval should be no greater than 100,000 years.

First the subroutine opens the temporary data file (**temp.dat**) created by the **CullDataPoints** subroutine and creates a new temporary data file (**temp2.dat**).

A **do-loop** is used to cycle through all of the time histories. The current time history is read from **temp.dat** and stored in the dynamically allocated **TempStorage** array.

A nested do-loop is then used to cycle through all of the rows in the current time history.

First the time for the current row of data is checked to see if it is greater than 50,000 years and less than 200,000 years. If so, the interval between it and the next time step is evaluated to determine if it is greater than 10,000 years. If so, the current row of data is written to the **temp2.dat** file, and the **AddPoints1** subroutine is called to generate a sufficient number of 10,000 year-spaced interpolated data sets such that no time interval is greater than 10,000 years. If the time interval is less than 10,000 years, the current row of data is written to the **temp2.dat** file.

Next the subroutine checks to see if the time history is greater than 200,000 years. If so, the interval between it and the next time step is checked to determine if it is greater than 100,000 years. If so, the current row of data is written to the **temp2.dat** file and the **AddPoints2** subroutine is called to generate a sufficient number of 100,000 year-spaced interpolated data sets such that no time interval is greater than 100,000 years. If the time interval is less than 100,000 years, the current row of data is written to the **temp2.dat** file.

If the time history is less than 50,000 years, the data is written to the temp2.dat file.

This process is repeated until all rows up to the last one have been checked. When the last row of data is reached, it is written to the **temp2.dat** file.

2.3.15 Subroutine AddPoints1

This subroutine interpolates data between time steps. It begins by checking to see if the time for the next row of data is greater than 200,000 years. If not, it skips forward to generate points for 10,000 year intervals. If so, it then sets two time steps, one for less than 200,000 years (**delTime1** = 200,000 years – current time step) and one for greater than 200,000 years (**delTime2** = 800,000 years). It then calculates the number of extra time steps needed for less than 200,000 years (**numExtraPoints1**) by dividing **delTime1** by 10,000 years. The number of time steps required above 200,000 years (**numExtraPoints2**) is determined by dividing **delTime2** by 100,000 years.

If **numExtraPoints1** is greater than zero, a **do-loop** is initiated that interpolates data points at 10,000 year intervals and writes them to the **TempStorage** array.

If **numExtraPoints2** is greater than zero, a **do-loop** is initiated that interpolates data points at 100,000 year intervals and writes them to the **TempStorage** array.

If the time step checked at the beginning of the routine is less than 200,000 years this, section of the subroutine calculates the time interval between the current time history and the next time history (**delTime**). It then divides **delTime** by 10,000 years to determine **numExtraPoints**. Next a **do-loop** is initiated that interpolates data points at 10,000 year intervals and writes them to the **TempStorage** array.

2.3.16 Subroutine AddPoints2

This subroutine interpolates data for time steps above 200,000 years. It begins by calculating the time interval between the current time step and the next time step (**delTime**). It then divides **delTime** by 100,000 years to determine **numExtraPoints**. Next a **do-loop** is initiated that interpolates data points at 100,000 year intervals and writes them to the **TempStorage** array.

2.3.17 Subroutine WriteOutputFile

This subroutine writes the output file from the **PREWAP** routine. It begins by opening the current output file (**outfile**) and the **temp2.dat** file. It then writes the initial comment lines and number of data sets to **outfile**. A **do-loop** is used to write each data set to the **outfile**. Within the **do-loop** the number of rows of data, the fraction of packages this data set is applicable to, and the header line for the data set are written to the **outfile**. Then a nested **do-loop** is used to read the data-set values from the **temp2.dat** file and write them to the **outfile**.

Finally the subroutine closes the **outfile** and **temp2.dat** files.

2.3.18 Subroutine DeallocateArrays

This subroutine deallocates all of the arrays allocated at the beginning of the program.

2.4 DESCRIPTION OF TEST CASES

PREWAP was validated using EXCEL spreadsheets to replicate PREWAP calculations and logic functions.

The interpolation subroutines were verified by running them independently of the overall program. A separate program was written containing the interpolate subroutines. This program was then compiled and run using an input deck that exercised all of the subroutine's calculations and logic functions. The output was written to output file. These results were then compared to an EXCEL spreadsheet that replicated the subroutine's calculations. These files are presented in Section 3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT. Visual inspections of these files show that the outputs from both methods agree, thus validating the operation of the interpolation subroutines.

Next the overall program was verified by comparing the output from the program using a limited input deck covering the full range of values expected for the input to the output from an EXCEL spreadsheet that replicated the programs calculations and logic functions. This was accomplished by copying the test data input file to an EXCEL spreadsheet. Additional columns were then added to the spreadsheet containing equations or logic functions performed by the PREWAP program. This included columns for intermediate and final output. The output from the PREWAP program, using the test file as input, was compared to the results obtained from the spreadsheet. These files are presented in Section 3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT. Visual inspection of these files shows that the output from the PREWAP program is consistent with the results generated by the spreadsheet.

2.5 DESCRIPTION OF TEST RESULTS

The results of these tests demonstrate that the output from the PREWAP program agrees with the test cases, verifying that the program correctly performs its intended functions.

2.6 RANGE OF INPUT VALUES FOR WHICH RESULTS WERE VERIFIED

Inputs to PREWAP are those physical parameters contained in the pH, Cl, and T-H files. Ranges for these parameters are those that are physically plausible for the parameter. For example RH cannot exceed 100%, pH and Cl concentrations values cannot be negative. No other limitations exist on the range of input parameter values.

2.7 LIMITATIONS ON SOFTWARE ROUTINE APPLICATIONS OR VALIDITY

This is a stand alone executable program that can be run under the Windows 95/98 and Windows NT operating environments on any PC platform with 100 megabytes of disk space and 64 megabytes of RAM.

3. SUPPORTING INFORMATION:

3.1 DIRECTORY LISTING OF EXECUTABLE AND DATA FILES

The PREWAP executable and the associated input files must be contained in the same directory. There are no other restrictions on directory names or structure that will affect the operation of the code.

3.2 COMPUTER LISTING OF SOURCE CODE

```
program prewap

! define dynamic variables
real(8), allocatable :: etime(:,:), wpT(:,:), dsT(:,:), dwT(:,:), iT(:,:)
real(8), allocatable :: wpRH(:,:), dsRH(:,:), dwRH(:,:), bfRH(:,:), iRH(:,:)
real(8), allocatable :: dsLS(:,:), iLS(:,:), massFracAir(:,:)
real(8), allocatable :: dwFluxWV(:,:), dwFluxAir(:,:)
real(8), allocatable :: dsEvapRate(:,:), bfEvapRate(:,:), iEvapRate(:,:)
real(8), allocatable :: PercFlux5m(:,:), tdsPercFlux(:,:), iPercFlux(:,:)
real(8), allocatable :: tdsT(:,:)

real(8), allocatable :: fract(:)

real(8), allocatable :: wpPHnd(:,:), wpCLnd(:,:), wpPHd(:,:), wpCLd(:,:)
real(8), allocatable :: dsPHnd(:,:), dsCLnd(:,:), dsPHd(:,:), dsCLd(:,:)
real(8), allocatable :: ipkPHnd(:,:), ipkCLnd(:,:), ipkPHd(:,:), ipkCLd(:,:)
real(8), allocatable :: barPHnd(:,:), barCLnd(:,:), barPHd(:,:), barCLd(:,:)

real(8), allocatable :: TempStorage(:,:)

integer(4), allocatable :: nRows(:), nnRows(:), nnnRows(:)

! define fixed variables

real(8) RHvector(10), Qvector(7), Tvector3(3), Tvector4(4), fCO2vector(7)
real(8) CLtable1a(10), CLtable1b(10), CLtable1c(10)
real(8) CLtable2a(7), CLtable2b(7)
real(8) CLtable3(7,3)
real(8) PHtable1a(10), PHtable1b(10), PHtable1c(10)
real(8) PHtable2a(7), PHtable2b(7)
real(8) PHtable3(7,3)
real(8) PHtable4(7,4)

real(8) ReadVector(22)
real(8) newValue(22)
```

```
integer(4) nRowsTable1, nRowsTable2, nRowsTable3, nColsTable3
integer(4) nRowsTable4, nColsTable4

real(8) ipkPHbounding, CorLim

integer(4) i, j, k
integer(4) iFile, nFile
integer(4) rows, maxRows, nDataSets, maxnnRows
integer(4) corFlag

character*6 dummy1
character*6 dummy2(6)
character*25 infile, outfile
character*25 InFileNames(100)
character*25 OutFileNames(100)

open(unit=99, file='debug.dat')        ! open debug file

! read in TH input and WAPDEG output file names
call ReadMasterFiles

! read in data for in-drift chemistry lookup tables
call ReadInDriftChemData

maxnnRows=0       ! initialize counter

! main program loop
! calls the subroutines that read in TH data, perform the necessary
! calculations, and generate the WAPDEG input files
do iFile=1,nFile

 ! screen for 'dummy' file names
 if (InFileNames(iFile) .ne. 'dummy') then
  infile=InFileNames(iFile)
  outfile=OutFileNames(iFile)

  write(*,*) "processing file: ", infile

  call CountDataSets
  call AllocateArrays
  call ReadInputFile
  call DoCalculations
  call CullDataPoints
  call AddDataPoints
  call WriteOutputFile
  call DeallocateArrays

 end if

end do

write(99,*) maxnnRows

close(99)    ! close debug file
```

```
contains

! this is the end of the "prewap" main program logic

! subroutines between the "contains" line and the "end subroutine prewap"
! line are internal to the "prewap" main program

!******************************************************************************
!******************************************************************************
subroutine ReadMasterFiles

! open 'InMaster.in' and 'OutMaster.in' files
open(unit=11, file='InMaster.in')
open(unit=12, file='OutMaster.in')

! read in the RH corrosion limit
read(11,*) CorLim

! read in the number of file names in the files
read(11,*) nFile

! read in input and output file names
do i=1,nFile
 read(11,*) InFileNames(i)
 read(12,*) OutFileNames(i)
end do

! close files
close(unit=11)
close(unit=12)

end subroutine ReadMasterFiles
!******************************************************************************
!******************************************************************************
subroutine ReadInDriftChemData

! read in log[Cl] data as a function of RH
open(unit=80, file='CLtable1.dat')
read(80,*) nRowsTable1      ! number of rows in the table
do m=1,nRowsTable1
 read(80,*) RHvector(m), CLtable1a(m), CLtable1b(m), CLtable1c(m)
end do
close(80)

! read in log[Cl] data as a function of 1-Qe/Qs
open(unit=80, file='CLtable2.dat')
read(80,*) nRowsTable2      ! number of rows in the table
do m=1,nRowsTable2
 read(80,*) Qvector(m), CLtable2a(m), CLtable2b(m)
end do
close(80)

! log[Cl] data as a function of 1-Qe/Qs and temperature(C)
open (unit=80, file='CLtable3.dat')

! number of rows and columns in the table
```

```
read(80,*) nRowsTable3, nColsTable3

! read in the temperature data
read(80,*) (Tvector3(n), n=1,nColsTable3)
do m=1,7
 read(80,*) Qvector(m), (CLtable3(m,n), n=1,nColsTable3)
end do
close(80)

! pH data as a function of RH
open(unit=80, file='PHtable1.dat')
do m=1,10
 read(80,*) RHvector(m), PHtable1a(m), PHtable1b(m), PHtable1c(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs
open(unit=80, file='PHtable2.dat')
do m=1,nRowsTable2
 read(80,*) Qvector(m), PHtable2a(m), PHtable2b(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs and temperature(C)
open (unit=80, file='PHtable3.dat')
read(80,*) (Tvector3(n), n=1,nColsTable3)
do m=1,nRowsTable3
 read(80,*) Qvector(m), (PHtable3(m,n), n=1,nColsTable3)
end do
close(80)

! pH data as a function of fCO2 and temperature(C)
open (unit=80, file='PHtable4.dat')
read(80,*) nRowsTable4, nColsTable4
read(80,*) (Tvector4(n), n=1,nColsTable4)
do m=1,nRowsTable4
 read(80,*) fCO2vector(m), (PHtable4(m,n), n=1,nColsTable4)
end do
close(80)


end subroutine ReadInDriftChemData
!******************************************************************************
!******************************************************************************
subroutine CountDataSets

open(unit=70, file=infile)

nDataSets=1               ! initialize # of data sets to 1
maxRows=0                 ! initialize the max number of rows to 0

! read past 1st four rows of header information
do i=1,4
 read(70,*) dummy1
end do
```

```
! read past header info in line 5 to get number of rows of data
read(70,*) (dummy2(i), i=1,5), rows
write(99,*) rows, "  rows"

! set max number of rows equal to the # of rows in 1st data set
maxRows=rows

! read past next six rows of header information
do i=1,6
 read(70,*) dummy1
end do

! read past the 1st data set
do i=1,rows
 read(70,*) dummy
end do

! read through the rest of the file until the end of the file is reached
do

! read the 1st row header information for the next data set
! if this read occurs at the end of the file, the 'eof' error
! causes the do loop to be exited
 read(70,*,end=100) (dummy2(i), i=1,5), rows
 !write(99,*) rows, "  rows"

! if an 'eof' error did not occur, increment the data set counter
! and read through the given data set
 nDataSets=nDataSets+1

! if the # of rows in the current data set are greater than the current
! max rows value, set max rows equal to the # of rows in the current data set
 if (rows .gt. maxRows) then
  maxRows=rows
 end if

! read through the current data set
 do i=1,(6+rows)
  read(70,*) dummy1
 end do

end do

! line that the 'eof' error causes the do-loop to bails out to
100 continue

! close the data file
close(unit=70)

! write the number of data sets to debug.dat
write(99,*) nDataSets, "  # of data sets"

end subroutine CountDataSets
!******************************************************************************
!******************************************************************************
subroutine AllocateArrays
```

```
! set bounds on dynamic arrays whose size is dependent upon the current TH file
allocate (etime(1:maxRows, 1:nDataSets))
allocate (wpT(1:maxRows, 1:nDataSets))
allocate (dsT(1:maxRows, 1: nDataSets))
allocate (dwT(1:maxRows, 1:nDataSets))
allocate (iT(1:maxRows, 1:nDataSets))
allocate (wpRH(1:maxRows, 1:nDataSets))
allocate (dsRH(1:maxRows, 1:nDataSets))
allocate (dwRH(1:maxRows, 1:nDataSets))
allocate (bfRH(1:maxRows, 1:nDataSets))
allocate (iRH(1:maxRows, 1:nDataSets))
allocate (dsLS(1:maxRows, 1:nDataSets))
allocate (iLS(1:maxRows, 1:nDataSets))
allocate (massFracAir(1:maxRows, 1:nDataSets))
allocate (dwFluxWV(1:maxRows, 1:nDataSets))
allocate (dwFluxAir(1:maxRows, 1:nDataSets))
allocate (dsEvapRate(1:maxRows, 1:nDataSets))
allocate (bfEvapRate(1:maxRows, 1:nDataSets))
allocate (iEvapRate(1:maxRows, 1:nDataSets))
allocate (PercFlux5m(1:maxRows, 1:nDataSets))
allocate (tdsPercFlux(1:maxRows, 1:nDataSets))
allocate (iPercFlux(1:maxRows, 1:nDataSets))
allocate (tdsT(1:maxRows, 1:nDataSets))

allocate (nRows(1:nDataSets))
allocate (nnRows(1:nDataSets))
allocate (nnnRows(1:nDataSets))
allocate (fract(1:nDataSets))

end subroutine AllocateArrays
!*********************************************************************************
!*********************************************************************************
subroutine ReadInputFile

open(unit=70, file=infile)       ! open input file

j=1        ! column index for 1st data set

! read past 1st four rows of header information
do i=1,4
 read(70,*) dummy1
end do

! read past header info in line 5 to get number of rows of data
read(70,*) (dummy2(i), i=1,5), nRows(j)

! read past header info in line 6 to get "fraction of this history" value
read(70,*) (dummy2(i), i=1,6), fract(j)

! read past next five rows of header information
do i=1,5
 read(70,*) dummy1
end do

! read in data from 1st data set
```

```
do i=1, nRows(j)
 read(70,*) etime(i,j),       &      ! time [yr]
          wpT(i,j),          &  ! temperature - waste package [C]
                dsT(i,j),          &  ! temperature - drip shield [C]
                dwT(i,j),          & ! temperature - drift wall [C]
                iT(i,j),           &   ! temperature - invert [C]
                wpRH(i,j),         &     ! rel. humidity - waste package [-]
                dsRH(i,j),         &     ! rel. humidity - drip shield [-]
                dwRH(i,j),         &     ! rel. humidity - drift wall [-]
                bfRH(i,j),         &! rel. humidity - backfill [-]
                iRH(i,j),          &  ! rel. humidity - invert [-]
                dsLS(i,j),         &!
          iLS(i,j),         &   !
                massFracAir(i,j),  &  ! mass frac. air [
                dwFluxWV(i,j),     &  ! water vapor flux - drift wall [
                dwFluxAir(i,j),    &    ! air flux - drift wall [
                dsEvapRate(i,j),   & ! evap. rate - drip shield [m3/yr]
                bfEvapRate(i,j),   &  ! evap. rate - backfill [m3/yr]
                iEvapRate(i,j),    &
                PercFlux5m(i,j),   &  ! perc flux @ 5m [mm/yr]
                tdsPercFlux(i,j),  &   ! perc flux -  drip shield top [mm/yr]
                iPercFlux(i,j),    &     ! perc flux - invert [mm/yr]
                tdsT(i,j)                ! temperature -  drip shield top [C]
end do

! now read in data for data sets 2 to nDataSets
do j=2,nDataSets

! read past header info in line 5 to get number of rows of data
 read(70,*) (dummy2(i), i=1,5), nRows(j)

! read past header info in line 6 to get "fraction of this history" value

 read(70,*) (dummy2(i), i=1,6), fract(j)

! read past next five rows of header information
 do i=1,5
  read(70,*) dummy1
 end do

! read in data from the j-th data set
 do i=1, nRows(j)
  read(70,*) etime(i,j),                              &
           wpT(i,j), dsT(i,j), dwT(i,j), iT(i,j),                &
           wpRH(i,j), dsRH(i,j), dwRH(i,j), bfRH(i,j), iRH(i,j),  &
           dsLS(i,j), iLS(i,j),                               &
           massFracAir(i,j),                                  &
           dwFluxWV(i,j), dwFluxAir(i,j),                        &
           dsEvapRate(i,j), bfEvapRate(i,j), iEvapRate(i,j),      &
                PercFlux5m(i,j), tdsPercFlux(i,j), iPercFlux(i,j),     &
                tdsT(i,j)
 end do

end do

close(unit=70)         ! close the data file
```

```
end subroutine ReadInputFile
!*******************************************************************************
!*******************************************************************************
subroutine DoCalculations

allocate (wpPHnd(1:maxRows, 1:nDataSets))
allocate (wpCLnd(1:maxRows, 1:nDataSets))

allocate (wpPHd(1:maxRows, 1:nDataSets))
allocate (wpCLd(1:maxRows, 1:nDataSets))

allocate (dsPHnd(1:maxRows, 1:nDataSets))
allocate (dsCLnd(1:maxRows, 1:nDataSets))

allocate (dsPHd(1:maxRows, 1:nDataSets))
allocate (dsCLd(1:maxRows, 1:nDataSets))

allocate (ipkPHnd(1:maxRows, 1:nDataSets))
allocate (ipkCLnd(1:maxRows, 1:nDataSets))

allocate (ipkPHd(1:maxRows, 1:nDataSets))
allocate (ipkCLd(1:maxRows, 1:nDataSets))

allocate (barPHnd(1:maxRows, 1:nDataSets))
allocate (barCLnd(1:maxRows, 1:nDataSets))

allocate (barPHd(1:maxRows, 1:nDataSets))
allocate (barCLd(1:maxRows, 1:nDataSets))

! perform calculations at each "i" time for all "j" data sets
do j=1,nDataSets
 do i=1,nRows(j)

! NOTE: CL chemistry is NOT calculated in this code version. Instead, pH^2 is
! reported in the wpCLd, wpCLnd, dsCLd, and dsCLnd variables

! calculate waste package in-drift pH and pH^2 for drip and no drip conditions
  call InDriftCalc(etime(i,j), wpT(i,j), wpRH(i,j),           &
                dsEvapRate(i,j), tdsPercFlux(i,j),         &
                        RHvector, Qvector, Tvector3, Tvector4,      &
                CLtable1a, CLtable1b, CLtable1c,           &
                CLtable2a, CLtable2b,                      &
                CLtable3,                              &
                PHtable1a, PHtable1b, PHtable1c,           &
                PHtable2a, PHtable2b,                      &
                PHtable3, PHtable4,                        &
                nRowsTable1, nRowsTable2,                  &
                        nRowsTable3, nColsTable3,                  &
                        nRowsTable4, nColsTable4,                  &
                        wpPHd(i,j), wpCLd(i,j), wpPHnd(i,j), wpCLnd(i,j),  &
                        i, j, infile)

! calculate drip shield in-drift pH and pH^2 for drip and no drip conditions
  call InDriftCalc(etime(i,j), dsT(i,j), dsRH(i,j),           &
                dsEvapRate(i,j), tdsPercFlux(i,j),         &
```

```
                    RHvector, Qvector, Tvector3, Tvector4,      &
                CLtable1a, CLtable1b, CLtable1c,          &
                CLtable2a, CLtable2b,                    &
                CLtable3,                           &
                PHtable1a, PHtable1b, PHtable1c,          &
                PHtable2a, PHtable2b,                    &
                PHtable3, PHtable4,                      &
                    nRowsTable1, nRowsTable2,               &
                    nRowsTable3, nColsTable3,              &
                    nRowsTable4, nColsTable4,              &
                    dsPHd(i,j), dsCLd(i,j), dsPHnd(i,j), dsCLnd(i,j),  &
                    i, j, infile)

! set bounding in-package pH for CSNF or HLW
if (infile(1:4) .eq. 'CSNF') then
 ipkPHbounding=7.60          ! CSNF bounding pH value
else
 ipkPHbounding=9.83          ! HLW bounding pH value
end if

! in-package drip pH is set equal to bounding values

  ipkPHd(i,j)=ipkPHbounding
  ipkCLd(i,j)=ipkPHd(i,j)*ipkPHd(i,j)
!  ipkCLd(i,j)=2.014E-04             ! mol/kg

! in-package no drip pH is set equal to -9.99E-02
! (default 'don't exist' values)
  ipkPHnd(i,j)=-9.99E-02
  ipkCLnd(i,j)=ipkPHnd(i,j)*ipkPHnd(i,j)

! barrier drip and no drip pH are set equal to -9.99E-02
! (default 'don't exist' values)
  barPHd(i,j)=-9.99E-02
  barCLd(i,j)=barPHd(i,j)*barPHd(i,j)
  barPHnd(i,j)=-9.99E-02
  barCLnd(i,j)=barPHnd(i,j)*barPHnd(i,j)

 end do
end do

end subroutine DoCalculations
!*******************************************************************************
!*******************************************************************************
subroutine CullDataPoints

open(unit=72, file='temp.dat')          ! open temporary storage file

! loop through all of the data sets
do j=1,nDataSets

 ! initialize counter for number of rows that will get written
 ! to temporary storage file
 nnRows(j)=0

 do i=1,nRows(j)-1
```

```
 corFlag=0       ! initialize corrosion flag to 0 (no corrosion)

 ! skip row if wpT or dsT 'do not exist'
 if(wpT(i,j) .le. 0.0 .or. dsT(i,j) .le. 0.0) then
  ! write to debug file
  !write(99,*) etime(i,j), "  trapped on no wpT or dsT"

 ! write row if wpRH or dsRH is equal or above corrosion limit
 elseif( (wpRH(i,j) .ge. CorLim) .or. (dsRH(i,j) .ge. CorLim) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  RH above corrosion limit"

 ! write row for wp no corrosion/corrosion transition
 elseif( (wpRH(i,j) .lt. 0.501) .and. (wpRH(i+1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  wp no cor/cor transition"

 ! write row for ds no corrosion/corrosion transition
 elseif( (dsRH(i,j) .lt. 0.501) .and. (dsRH(i+1,j) .ge. 0.501)  ) then
  corFlag=1
  !write(99,*) etime(i,j), "  ds no cor/cor transition"

 ! write row for wp corrosion/no corrosion transition
 elseif( (wpRH(i,j) .lt. 0.501) .and. (wpRH(i-1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  wp cor/no cor transition"

 ! write row for ds corrosion/no corrosion transition
 elseif( (dsRH(i,j) .lt. 0.501) .and. (dsRH(i-1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  ds cor/no cor transition"

 ! skip row if in middle of no corrosion
 elseif( (wpRH(i,j) .lt. 0.501) .and.  &
        (wpRH(i-1,j) .lt. 0.501) .and.  &
        (wpRH(i+1,j) .lt. 0.501) ) then

  !write(99,*) etime(i,j), "  trapped on middle of no corrosion (wp)"
  ! trap

 elseif( (dsRH(i,j) .lt. 0.501) .and.  &
        (dsRH(i-1,j) .lt. 0.501) .and.  &
            (dsRH(i+1,j) .lt. 0.501) ) then

  !write(99,*) etime(i,j), "  trapped on middle of no corrosion (ds)"
  ! trap

 else
! middle of corrosion
  corFlag=1
  !write(99,*) etime(i,j), "  default"

 end if

 ! write the i-th row of data to the temp file if corFlag=1
```

```
  if(corFlag .eq. 1) then
   write(72,1020) etime(i,j), wpT(i,j), wpRH(i,j), dsT(i,j), dsRH(i,j),   &
            wpPHnd(i,j), wpCLnd(i,j), wpPHd(i,j), wpCLd(i,j),      &
                  dsPHnd(i,j), dsCLnd(i,j), dsPHd(i,j), dsCLd(i,j),      &
                  ipkPHnd(i,j), ipkCLnd(i,j), ipkPHd(i,j), ipkCLd(i,j),  &
                  barPHnd(i,j), barCLnd(i,j), barPHd(i,j), barCLd(i,j),  &
                  PercFlux5m(i,j)
   1020 format(22(ES10.3, "  "))

   ! increment the number of rows stored for the j-th time history
   nnRows(j)=nnRows(j)+1

  end if

 end do

 ! write the last time history to the temp file
 i=nRows(j)
 write(72,1020) etime(i,j), wpT(i,j), wpRH(i,j), dsT(i,j), dsRH(i,j),   &
            wpPHnd(i,j), wpCLnd(i,j), wpPHd(i,j), wpCLd(i,j),      &
                  dsPHnd(i,j), dsCLnd(i,j), dsPHd(i,j), dsCLd(i,j),      &
                  ipkPHnd(i,j), ipkCLnd(i,j), ipkPHd(i,j), ipkCLd(i,j),  &
                  barPHnd(i,j), barCLnd(i,j), barPHd(i,j), barCLd(i,j),  &
                  PercFlux5m(i,j)

 ! increment the number of rows stored for the j-th time history
 nnRows(j)=nnRows(j)+1

 write(99,*) j, nnRows(j)


 if(nnRows(j) .gt. maxnnRows) then
  maxnnRows=nnRows(j)
 end if

end do

close(72)

end subroutine CullDataPoints
!*******************************************************************************
!*******************************************************************************
subroutine AddDataPoints

open(unit=72, file='temp.dat')          ! open temporary storage files
open(unit=73, file='temp2.dat')


do j=1, nDataSets          ! loop through the time histories

  allocate (TempStorage(1:nnRows(j), 1:22))       ! set TempStorage array size

 ! initialize counter for number of rows to be written to the WAPDEG input file
 ! for the j-th time history
 nnnRows(j)=nnRows(j)
```

```
! read j-th time history from temp.dat file
do i=1,nnRows(j)
 read(72,*) (TempStorage(i,m), m=1,22)
end do

 do i=1,nnRows(j)-1! loop through all but the last row of data

 ! check times between 50,000 and 200,000 years to see
 ! if time steps are <= 10,000 years
 if((TempStorage(i,1) .ge. 50000.0)  .and.   &
    (TempStorage(i,1) .lt. 200000.0)) then

  ! if time step is greater than 10,000 years write current row of data
  ! to temp2.dat and call subroutine to add interpolated data and times
  ! at 10,000 year intervals between the i-th and i-th+1 rows
  if(TempStorage(i+1,1)-TempStorage(i,1) .gt. 10000.0) then
   write(73,1020) (TempStorage(i,m), m=1,22)
     1020 format(22(ES10.3, "  "))
   call AddPoints1

  else
   ! if time step is <= 10,000 years write current row of data to temp2.dat
   write(73,1020) (TempStorage(i,m), m=1,22)

  endif

 ! check times after 200,000 years to see
 ! if time steps are <= 100,000 years
 elseif(TempStorage(i,1) .ge. 200000.0) then

  ! if time step is greater than 100,000 years write current row of data
  ! to temp2.dat and call subroutine to add interpolated data and times
  ! at 100,000 year intervals between the i-th and i-th+1 rows
  if(TempStorage(i+1,1)-TempStorage(i,1) .gt. 100000.0) then
   write(73,1020) (TempStorage(i,m), m=1,22)
     call AddPoints2

  else
   ! if time step is <= 100,000 years write current row of data to temp2.dat
   write(73,1020) (TempStorage(i,m), m=1,22)

  endif

 else
 ! if time is <= 50,000 years write current row of data to temp2.dat
  write(73,1020) (TempStorage(i,m), m=1,22)

 endif

end do

! write the last row of data to the temp2.dat file
write(73,1020) (TempStorage(nnRows(j),m), m=1,22)

deallocate (TempStorage)        ! deallocate the TempStorage array
```

```
end do

close(72)          ! close temporary files
close(73)

end subroutine AddDataPoints
!******************************************************************************
!******************************************************************************
subroutine WriteOutputFile

open(unit=71, file=outfile)          ! open output file
open(unit=73, file='temp2.dat')  ! open temporary storage file

! write initial comment lines
write(71,1011)
1011 format('! 1st comment line')
write(71,1012)
1012 format('! 2nd comment line')
write(71,1013)
1013 format('! 3rd comment line')

write(71,1014) nDataSets
1014 format('# ', I4, '  21')     ! # of datasets and # of columns of data
                                          ! WAPDEG guys don't want 22nd column
do j=1,nDataSets
 write(71,1015) nnnRows(j)
 1015 format('# ', I4)            ! # of rows in the j-th dataset

 write(71,1016) fract(j)
 1016 format('# ', ES10.3)          ! fraction of packages

 write(71,1018)                         ! writes header line
 1018 format('!  t        ', '  wpT      ', '  wpRH     ',   &
           '  dsT      ', '  dsRH     ', '  wpPHnd    ',    &
                '  wpCLnd    ', '  wpPHd     ', '  wpCLd     ',    &
                '  dsPHnd    ', '  dsCLnd    ', '  dsPHd     ',    &
                '  dsCLd     ', '  ipkPHnd   ', '  ipkCLnd   ',    &
                '  ipkPHd    ', '  ipkCLd    ', '  barPHnd   ',    &
                '  barCLnd   ', '  barPHd    ', '  barCLd    ',    &
              '  PercFlux5m')

 1020 format(22(ES10.3, "  "))
 do i=1,nnnRows(j)
  read(73,*) (ReadVector(m), m=1,22)
  write(71,1020) (ReadVector(m), m=1,22)
 end do


end do

write(99,*)

close(unit=71)        ! close output file
close(unit=73)        ! close temporary storage file

end subroutine WriteOutputFile
```

```
!******************************************************************************
!******************************************************************************
subroutine DeallocateArrays

! deallocate arrays
deallocate (etime, wpT,  dsT, dwT, iT, wpRH, dsRH, dwRH, bfRH, iRH)
deallocate (dsLS, iLS, massFracAir, dwFluxWV, dwFluxAir)
deallocate (dsEvapRate, bfEvapRate, iEvapRate)
deallocate (PercFlux5m, tdsPercFlux, iPercFlux, tdsT)

deallocate (fract)

deallocate (wpPHnd, wpCLnd, wpPHd,  wpCLd)
deallocate (dsPHnd,  dsCLnd,  dsPHd, dsCLd)
deallocate (ipkPHnd,  ipkCLnd,  ipkPHd,  ipkCLd)
deallocate (barPHnd,  barCLnd,  barPHd,  barCLd)

deallocate (nRows, nnRows, nnnRows)

end subroutine DeallocateArrays
!******************************************************************************
!******************************************************************************
subroutine AddPoints1

! check for time step spanning across 200,000 years
if (TempStorage(i+1,1) .gt. 200000.0) then
 ! if it does set two time steps
 ! one for <= 200,000 and one for > 200,000 years
 delTime1=200000.0-TempStorage(i,1)
 delTime2=800000.0

 ! calculate the number of extra points to be added
 numExtraPoints1 = ceiling(delTime1/10000)
 numExtraPoints2 = ceiling(delTime2/100000)-1


 if (numExtraPoints1 .ne. 0) then
 ! generate interpolated data for the extra points to be added
  do ii=1,numExtraPoints1
   do jj=2,22
    delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
    newValue(jj)=TempStorage(i,jj) + delDep*(10000*ii/delTime1)
   end do
   1021 format(22(ES10.3, "  "))
   ! write the interpolated data to the temp2.dat file
   write(73,1021) TempStorage(i,1)+10000*ii, (newValue(m), m=2,22)
  end do
 end if

 if (numExtraPoints2 .ne. 0) then
  ! generate interpolated data for the 1st extra point to be added
  do jj=2,22
   delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
   newValue(jj)=TempStorage(i,jj) +  &
              delDep*(200000-TempStorage(i,1))/(TempStorage(i+1,1)-TempStorage(i,1))
  end do
```

```
  ! write the interpolated data to the temp2.dat file
  write(73,1021) 300000.0, (newValue(m), m=2,22)

  ! generate interpolated data for the remaining extra points to be added
  do ii=2,numExtraPoints2
   do jj=2,22
    delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
    newValue(jj)=TempStorage(i,jj) + delDep*(100000*ii/delTime2)
   end do
   ! write the interpolated data to the temp2.dat file
   write(73,1021) 200000.0+100000.0*ii, (newValue(m), m=2,22)
  end do
 end if

 ! increment the number of rows of the j-ht time history by the number of points added
 nnnRows(j)=nnnRows(j)+numExtraPoints1+numExtraPoints2

else
 ! time step doesn't span 200,000 years

 ! calculate the number of extra points to be added
 delTime=TempStorage(i+1,1)-TempStorage(i,1)
 numExtraPoints = ceiling(delTime/10000)-1

 if (numExtraPoints .eq. 0) then
  return
 end if

 ! generate interpolated data for the points to be added
 do ii=1,numExtraPoints
  do jj=2,22
   delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
   newValue(jj)=TempStorage(i,jj) + delDep*(10000*ii/delTime)
  end do
  ! write the interpolated data to the temp2.dat file
  write(73,1021) TempStorage(i,1)+10000*ii, (newValue(m), m=2,22)
 end do

 ! increment the number of rows of the j-ht time history by the number of points added
 nnnRows(j)=nnnRows(j)+numExtraPoints

end if

end subroutine AddPoints1
!*******************************************************************************
!*******************************************************************************
subroutine AddPoints2

delTime=TempStorage(i+1,1)-TempStorage(i,1)

numExtraPoints = ceiling(delTime/100000)-1

if (numExtraPoints .eq. 0) then
 return
end if
```

```
do ii=1,numExtraPoints
 do jj=2,22
  delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
  newValue(jj)=TempStorage(i,jj) + delDep*(100000*ii/delTime)
 end do
 write(73,1022) TempStorage(i,1)+100000*ii, (newValue(m), m=2,22)
 1022 format(22(ES10.3, "  "))
end do

nnnRows(j)=nnnRows(j)+numExtraPoints

end subroutine AddPoints2
!*****************************************************************************
!*****************************************************************************
end program prewap

! subroutines past this point are external to the "prewap" main program

!*****************************************************************************
!*****************************************************************************
! calualate the pH and Cl under drip and no drip conditions

! NOTE: CL chemistry is NOT calculated in this code version. Instead, pH^2 is
! reported in the wpCLd, wpCLnd, dsCLd, and dsCLnd variables

subroutine InDriftCalc(etime, T, RH, EvapRate, SeepRate,      &
                  RHvector, Qvector, Tvector3, Tvector4,     &
              CLtable1a, CLtable1b, CLtable1c,          &
              CLtable2a, CLtable2b,                    &
              CLtable3,                          &
              PHtable1a, PHtable1b, PHtable1c,          &
              PHtable2a, PHtable2b,                    &
              PHtable3, PHtable4,                      &
                  nRowsTable1, nRowsTable2,                &
                  nRowsTable3, nColsTable3,                &
                  nRowsTable4, nColsTable4,                &
              PHd, CLd, PHnd, CLnd,                    &
                i, j, infile)

real(8) RHvector(nRowsTable1), Qvector(nRowsTable2), fCO2vector(nRowsTable4)
real(8) Tvector3(nColsTable3), Tvector4(nColsTable4)
real(8) CLtable1a(nRowsTable1), CLtable1b(nRowsTable1), CLtable1c(nRowsTable1)
real(8) CLtable2a(nRowsTable2), CLtable2b(nRowsTable2)
real(8) CLtable3(nRowsTable3,nColsTable3)
real(8) PHtable1a(nRowsTable1), PHtable1b(nRowsTable1), PHtable1c(nRowsTable1)
real(8) PHtable2a(nRowsTable2), PHtable2b(nRowsTable2)
real(8) PHtable3(nRowsTable3,nColsTable3)
real(8) PHtable4(nRowsTable4,nColsTable4)

real(8) etime, T, RH, Qratio, EvapRate, SeepRate
real(8) PHd, CLd, PHnd, CLnd, logCLd, logfCO2

integer(4) nRowsTable1, nRowsTable2, nRowsTable3, nColsTable3
integer(4) i, j

character*15 infile
```

```
! trap for temperatures and seep rates that "don't exist"
if( (T .lt. 0.0) .or. (SeepRate .lt. -99.0)) then

! drip and no drip pH are set equal to -9.99E-02
! (default 'don't exist' values)
 PHd=-9.99E-02
 PHnd=-9.99E-02

! place holder for CL calculations
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

else

! calculate 1-Qe/Qs
 if( SeepRate .eq. 0.0) then        ! sets 1-Qe/Qs equal to 0.0 when Qs=0
  Qratio=0.0
 else
  Qratio=1.0 - abs(EvapRate/SeepRate)
 end if

! determine what range of in-drift chemistry data is applicable, then
! calculate pH and pH^2

! 1st period (< 50 years -- pre-closure) ************************************
 if(etime .lt. 50.0) then

  ! drip and no drip pH are set equal to -9.99E-02
  ! (default 'don't exist' values)
  PHd=-9.99E-02
  PHnd=-9.99E-02

! place holder for CL calculations
   ! drip and no drip CL are set equal to -9.99E-02
   ! (default 'don't exist' values)
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

! 2nd time period (50 to 1000 years) ***************************************
 elseif( (etime .gt. 50.0) .and. (etime .le. 1000.0) ) then

  logfCO2=-6.5

  ! 1st range (RH <= 50)
  if (100*RH .le. 50.0) then
   !!write(99,*) "1st range"

   ! drip and no drip pH are set equal to -9.99E-02
   ! (default 'don't exist' values)
   PHd=-9.99E-02
   PHnd=-9.99E-02

! place holder for CL calculations
   ! drip and no drip CL are set equal to -9.99E-02
   ! (default 'don't exist' values)
```

```
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

  ! 2nd range (50 <= RH <= 85)
  elseif( (100*RH .ge. 50.0) .and.  &
        (100*RH .le. 85.0) ) then

   !!write(99,*) "2nd range"

   PHd=9.40      ! drip pH is constant in this range
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
             nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(100*RH, RHvector, CLtable1a, nRowsTable1, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  ! 3rd range (RH > 85)
  elseif(100*RH .gt. 85.0) then

   !!write(99,*) "3rd range"

   call Interp1D(Qratio, Qvector, PHtable2a, nRowsTable2, PHd)
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
             nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(Qratio, Qvector, CLtable2a, nRowsTable2, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  else
   !!write(99,*) "failed all 2nd period tests"
  end if

 ! 3rd time period (1000 years to 2000 years) *************************
 elseif( (etime .gt. 1000.0) .and. (etime .le. 2000.0) ) then

  logfCO2=-3.0

 ! 1st range (RH < 50)
  if (100*RH .lt. 50.0) then
   !!write(99,*) "1st range"

   ! drip and no drip pH are set equal to -9.99E-02
   ! (default 'don't exist' values)
   PHd=-9.99E-02
   PHnd=-9.99E-02

! place holder for CL calculations
   ! drip and no drip CL are set equal to -9.99E-02
   ! (default 'don't exist' values)
!   CLd=-9.99E-02
!   CLnd=-9.99E-02
```

```
  ! 2nd range (50 <= RH <= 85)
  elseif( (100*RH .ge. 50.0) .and.  &
         (100*RH .le. 85.0) ) then

   !!write(99,*) "2nd range"


   PHd=7.64       ! drip pH is constant in this range
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  ! 3rd range (RH > 85)
  elseif(100*RH .gt. 85.0) then

   !!write(99,*) "3rd range"
   call Interp1D(Qratio, Qvector, PHtable2b, nRowsTable2, PHd)
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(Qratio, Qvector, CLtable2b, nRowsTable2, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  else
   !!write(99,*) "failed all 3nd period tests"
  end if

 ! 4th time period (2000 year to 100,000 years) *******************
 elseif( (etime .gt. 2000.0) .and. (etime .le. 100000.0) ) then

  logfCO2=-2.0

  ! 1st range (RH < 50)
  if (100*RH .lt. 50.0) then
   !!write(99,*) "1st range"

   PHd=-9.99E-02
   PHnd=-9.99E-02

! place holder for CL calculations
!   CLd=-9.99E-02
!   CLnd=-9.99E-02

  ! 2nd range (50 <= RH <= 85)
  elseif( (100*RH .ge. 50.0) .and.  &
        (100*RH .le. 85.0) ) then

   !!write(99,*) "2nd range"

   PHd=7.02       ! drip pH is constant in this range
```

```
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  ! 3rd range (RH > 85)
  else

   !!write(99,*) "3rd range"

   call Interp2D(Qratio, T, Qvector, Tvector3, PHtable3, &
             nRowsTable3, nColsTable3, PHd)
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp2D(Qratio, T, Qvector, Tvector, CLtable3, &
!               nRowsTable3, nColsTable3, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  end if

 ! 5th time period (>100,000 years) *******************
 else

  logfCO2=-3.0

  ! 1st range (RH < 50)
  if (100*RH .lt. 50.0) then
   !!write(99,*) "1st range"

   PHd=-9.99E-02
   PHnd=-9.99E-02

! place holder for CL calculations
!   CLd=???
!   CLnd=-9.99E-02

  ! 2nd range (50 <= RH <= 85)
  elseif( (100*RH .ge. 50.0) .and.  &
       (100*RH .le. 85.0) ) then

   !!write(99,*) "2nd range"

   PHd=7.64       ! drip pH is constant in this range
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02
```

```
  ! 3rd range (RH > 85)
  elseif(100*RH .gt. 85.0) then

   !!write(99,*) "3rd range"
   call Interp1D(Qratio, Qvector, PHtable2b, nRowsTable2, PHd)
   call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
              nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(Qratio, Qvector, CLtable2b, nRowsTable2, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

  end if

 end if

end if

! substitute pH^2 values in place of CL values
CLd=PHd*PHd
CLnd=PHnd*PHnd

  !!write(99,*) etime, " etime"
  !!write(99,*) j, i, " j-th dataset, i-th time"
  !!write(99,*) T, " temp"
  !!write(99,*) RH, " RH"
  !!write(99,*) EvapRate, " evap rate"
  !!write(99,*) SeepRate, " seep rate"
  !!write(99,*) Qratio, " Qe/Qs"
  !!write(99,*)

end subroutine InDriftCalc
!********************************************************************************
!********************************************************************************
! 1-D interpolation routine
subroutine Interp1D(ind, IndData, DepData, nRows, dep)

! number of rows in 1-D table
integer(4) nRows

! independent and dependent variable vectors
real(8) IndData(nRows), DepData(nRows)

! independent and dependent variables
real(8) ind, dep

! check for independent variable outside of data set range
if (ind .le. IndData(1)) then
 dep=DepData(1)                ! value is below lower bound, set equal to floor
elseif (ind .ge. IndData(nRows)) then
 dep=DepData(nRows)        ! value is above upper bound, set equal to ceiling
else

 do i=1,nRows-1           ! value is within the range of the data set
```

```
  if ((ind .ge. IndData(i)) .and. (ind .lt. IndData(i+1))) then

   ! linear interpolation
   ! y = y(i) + [x-x(i)]/[x(i+1)-x(i)] * [y(i+1)-y(i)]
   dep=DepData(i)  &
          + (ind-IndData(i))/(IndData(i+1)-IndData(i))  &
                *(DepData(i+1)-DepData(i))
  end if
 end do
end if

end subroutine Interp1D
!*******************************************************************************
!*******************************************************************************
subroutine Interp2D(ind1, ind2, IndData1, IndData2, DepData, nRows, nCols, dep)

! number of rows and columns in 2-D table
integer(4) nRows, nCols

! independent variable vectors and dependent variable array
real(8) IndData1(nRows), IndData2(nCols), DepData(nRows,nCols)

! independent variables, intermediate dependent variables, and dependent variable
real(8) ind1, ind2, dep1, dep, dep2

! flags for independent variable values beyond upper and lower bounds
integer(4) iflag_lb, iflag_ub, jflag_lb, jflag_ub

!!write(99,*) "in Interp2D"
!!write(99,*) ind1, " ind1"
!!write(99,*) ind2, " ind2"

! initialize flags
iflag_lb = 0
iflag_ub = 0
jflag_lb = 0
jflag_ub = 0

! determine i-index
if (ind1 .le. IndData1(1)) then
 i=1            ! ind1 less than lower bound
 iflag_lb = 1
elseif (ind1 .ge. IndData1(nRows)) then
 i=nRows          ! ind1 greater than upper bound
 iflag_ub = 1

else

 do ii=1,nRows-1
  if ((ind1 .ge. IndData1(ii)) .and. (ind1 .lt. IndData1(ii+1))) then
   i=ii           ! ind1 is between IndData1(ii) and IndData1(ii+1)
  end if
 end do

end if
```

```
!!write(99,*) i, " i"


! determine j-index
if (ind2 .le. IndData2(1)) then
 j=1             ! ind2 less than lower bound
 jflag_lb = 1

elseif (ind2 .ge. IndData1(nCols)) then
 j=nCols           ! ind2 greater than upper bound
 jflag_ub = 1

else

 do jj=1,nCols-1
  if ((ind2 .ge. IndData2(jj)) .and. (ind2 .lt. IndData2(jj+1))) then
   j=jj                 ! ind2 is between IndData2(jj) and IndData2(jj+1)
  end if
 end do

end if

!!write(99,*) j, " j"

! logic trap to catch points below the lower bound of the table
if(iflag_lb .eq. 1) then     ! outside lower bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
 dep=DepData(i,j)          ! corner point
 else
 ! linearly interpolate along lower edge
  dep=DepData(i,j)  &
     + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
         *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points above the upper bound of the table
if(iflag_ub .eq. 1) then    ! outside upper bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)         ! corner point
 else
 ! linearly interpolate along upper edge
  dep=DepData(i,j)  &
     + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
         *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points beyond the left and right bound of the table
if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
 ! outside right or left bound
 if( (iflag_lb .eq. 1) .or. (iflag_ub .eq. 1) ) then
  ! trap for corner points (already calculated)
 else
  ! linearly interpolate along left or right edge
  dep=DepData(i,j)  &
```

```
     + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
       *(DepData(i+1,j)-DepData(i,j))
 end if
end if

! logic trap to catch points in the table
if( (iflag_lb .eq. 0) .and. (iflag_ub .eq. 0) .and.  &
    (jflag_lb .eq. 0) .and. (jflag_ub .eq. 0) ) then

! interpolate in j-th column between the i-th and (i+1)-th row
dep1i=DepData(i,j)  &
    + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
      *(DepData(i+1,j)-DepData(i,j))

! interpolate in (j+1)-th column between the i-th and (i+1)-th row
dep2i=DepData(i,j+1)  &
    + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
      *(DepData(i+1,j+1)-DepData(i,j+1))

! interpolate the results above results between
! the j-th and (j+1)-th columns
dep=dep1i           &
  +(ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))     &
    *(dep2i-dep1i)

end if

end subroutine Interp2D
!*******************************************************************************
!*******************************************************************************
```

3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

3.3.1 Source Code For Testing The Interpolation Subroutines

```
program PWinterp

real(8) CLvector(10), CLtable1a(10)
real(8) Tvector(3), Qvector(7), PHtable3(7,3)
real(8) nInput1D, nInput2D
real(8) indVar1, indVar2
real(8) dep

integer(4) nRows1
integer(4) nRows2, nCols2

call ReadChemData

open(unit=90, file='input1D.dat')
open(unit=91, file='output1D.dat')
read(90,*) nInput1D
do i=1,nInput1D
```

```
 read(90,*) indVar1
 call Interp1D(indVar1, CLvector, CLtable1a, nRows1, dep)
 write(91,*) indVar1, dep
end do
close(90)
close(91)

open(unit=90, file='input2D.dat')
open(unit=91, file='output2D.dat')
read(90,*) nInput2D
do i=1,nInput2D
 read(90,*) indVar1, indVar2
 call Interp2D(indVar1, indVar2, Qvector, Tvector, PHtable3, nRows2, nCols2, dep)
 write(91,*) indVar1, indVar2, dep
end do
close(90)
close(91)

contains

!*******************************************************************************
subroutine ReadChemData

! CL data as a function of RH (1-D table)
open(unit=80, file='CLtable1.dat')
read(80,*) nRows1

do m=1,nRows1
 read(80,*) CLvector(m), CLtable1a(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs and temperature(C) (2-D table)
open (unit=80, file='PHtable3.dat')
read(80,*) nRows2, nCols2
read(80,*) (Tvector(n), n=1,nCols2)
do m=1,nRows2
 read(80,*) Qvector(m), (PHtable3(m,n), n=1,nCols2)
end do
close(80)

end subroutine ReadChemData
!*******************************************************************************

end program PWinterp

!*******************************************************************************
!*******************************************************************************
! 1-D interpolation routine
subroutine Interp1D(ind, IndData, DepData, nRows, dep)

! number of rows in 1-D table
integer(4) nRows

! independent and dependent variable vectors
real(8) IndData(nRows), DepData(nRows)
```

```
! independent and dependent variables
real(8) ind, dep

! check for independent variable outside of data set range
if (ind .le. IndData(1)) then
 dep=DepData(1)                 ! value is below lower bound, set equal to floor
elseif (ind .ge. IndData(nRows)) then
 dep=DepData(nRows)         ! value is above upper bound, set equal to ceiling
else

 do i=1,nRows-1            ! value is within the range of the data set
  if ((ind .ge. IndData(i)) .and. (ind .lt. IndData(i+1))) then

   ! linear interpolation
   ! y = y(i) + [x-x(i)]/[x(i+1)-x(i)] * [y(i+1)-y(i)]
   dep=DepData(i)  &
          + (ind-IndData(i))/(IndData(i+1)-IndData(i))  &
                *(DepData(i+1)-DepData(i))
  end if
 end do
end if

end subroutine Interp1D
!**********************************************************************************
!**********************************************************************************
subroutine Interp2D(ind1, ind2, IndData1, IndData2, DepData, nRows, nCols, dep)

! number of rows and columns in 2-D table
integer(4) nRows, nCols

! independent variable vectors and dependent variable array
real(8) IndData1(nRows), IndData2(nCols), DepData(nRows,nCols)

! independent variables, intermediate dependent variables, and dependent variable
real(8) ind1, ind2, dep1, dep, dep2

! flags for independent variable values beyond upper and lower bounds
integer(4) iflag_lb, iflag_ub, jflag_lb, jflag_ub

! initialize flags
iflag_lb = 0
iflag_ub = 0
jflag_lb = 0
jflag_ub = 0

! determine i-index
if (ind1 .le. IndData1(1)) then
 i=1             ! ind1 less than lower bound
 iflag_lb = 1
elseif (ind1 .ge. IndData1(nRows)) then
 i=nRows          ! ind1 greater than upper bound
 iflag_ub = 1

else
```

```
 do ii=1,nRows-1
  if ((ind1 .ge. IndData1(ii)) .and. (ind1 .lt. IndData1(ii+1))) then
   i=ii            ! ind1 is between IndData1(ii) and IndData1(ii+1)
  end if
 end do

end if

! determine j-index
if (ind2 .le. IndData2(1)) then
 j=1              ! ind2 less than lower bound
 jflag_lb = 1

elseif (ind2 .ge. IndData2(nCols)) then
 j=nCols            ! ind2 greater than upper bound
 jflag_ub = 1

else

 do jj=1,nCols-1
  if ((ind2 .ge. IndData2(jj)) .and. (ind2 .lt. IndData2(jj+1))) then
   j=jj                 ! ind2 is between IndData2(jj) and IndData2(jj+1)
  end if
 end do

end if

! logic trap to catch points below the lower bound of the table
if(iflag_lb .eq. 1) then     ! outside lower bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)         ! corner point

 else
 ! linearly interpolate along lower-bound edge
  dep=DepData(i,j)  &
     + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
          *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points above the upper bound of the table
if(iflag_ub .eq. 1) then    ! outside upper bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)         ! corner point
 else
 ! linearly interpolate along upper edge
  dep=DepData(i,j)  &
     + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
          *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points beyond the left and right bound of the table
if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
 ! outside right or left bound
 if( (iflag_lb .eq. 1) .or. (iflag_ub .eq. 1) ) then
```

```
  ! trap for corner points (already calculated)
 else
  ! linearly interpolate along left or right edge
  dep=DepData(i,j)  &
     + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
       *(DepData(i+1,j)-DepData(i,j))
 end if
end if

! logic trap to catch points in the table
if( (iflag_lb .eq. 0) .and. (iflag_ub .eq. 0) .and.  &
    (jflag_lb .eq. 0) .and. (jflag_ub .eq. 0) ) then

! interpolate in j-th column between the i-th and (i+1)-th row
dep1i=DepData(i,j)  &
    + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
      *(DepData(i+1,j)-DepData(i,j))

! interpolate in (j+1)-th column between the i-th and (i+1)-th row
dep2i=DepData(i,j+1)  &
    + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
      *(DepData(i+1,j+1)-DepData(i,j+1))

! interpolate the results above results between
! the j-th and (j+1)-th columns
dep=dep1i           &
  +(ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))     &
    *(dep2i-dep1i)

end if

end subroutine Interp2D
!*********************************************************************************
!*********************************************************************************
```

3.3.2 Input File For 1D Interpolation Subroutine Test Case

```
4
50.0
53.1
60.0
90.0

10
50.3     -2.431   -2.428   -2.415
51.0     -1.246   -1.244   -1.231
53.1     -0.389   -0.391   -0.380
55.2     -0.164   -0.169   -0.159
60.5     0.225          0.211          0.216
65.7     0.380          0.358          0.359
71.0     0.420          0.396          0.396
76.2     0.428          0.403          0.403
81.5     0.418          0.394          0.394
85.0     0.407          0.382          0.382
```

```
     2          3          4
; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))
```

3.3.3 Output File For 1D Interpolation Subroutine Test Case

```
50.0000000000000     -2.43100000000000
53.1000000000000     -0.389000000000000
60.0000000000000      0.188301886792453
90.0000000000000      0.407000000000000
```

3.3.4 EXCEL Spreadsheet Replicating 1D Interpolation Subroutine

1D Interpolation Subroutine				
Lookup Table			Interpolated Values	
Independent Variable	Dependent Variable		Independent Variable	Interpolated Value of Dependent Variable
50.3	-2.431		50	-2.43100
51	-1.246		53.1	-0.38900
53.1	-0.389		60	0.18830
55.2	-0.164		90	0.40700
60.5	0.225			
65.7	0.38			
71	0.42			
76.2	0.428			
81.5	0.418			
85	0.407			

3.3.5 Input File For 2D Interpolation Subroutine Test Case

```
9
0.0  20.0
0.0  80.0
1.1  20.0
1.1  80.0
0.2  20.0
0.2  80.0
0.0  65.0
1.1  65.0
45.0
```

3.3.6 2D Lookup Table

```
7    3
          25        50        75
0.0011999  7.02          7.02          7.02
0.0012  6.78          6.86          7.02
0.01         6.986        6.95          7.02
0.1       7.11          7.03          6.97
0.5       7.23          7.18          7.14
0.9       7.09          7.22          7.18
1.0       7.05          7.22          7.19
; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; condition: Period 4
; 1st independent variable (columns) = temperature ('C)
; dependent parameter = pH
```

3.3.7 Output File For 2D Interpolation Subroutine Test Case

```
000000000000000E+000     20.0000000000000       7.02000000000000
0.000000000000000E+000   80.0000000000000       7.02000000000000
1.10000000000000        20.0000000000000       7.05000000000000
1.10000000000000        80.0000000000000       7.19000000000000
0.200000000000000        20.0000000000000       7.14000000000000
0.200000000000000        80.0000000000000       7.01250000000000
0.000000000000000E+000   65.0000000000000       7.02000000000000
1.10000000000000        65.0000000000000       7.20200000000000
0.250000000000000        45.0000000000000       7.09999990463257
```

3.3.8 EXCEL Spreadsheet Replicating 2D Interpolation Subroutine

2D Interpolation Subroutine						
2D Lookup Table				Interpolated Value of Dependent Variable		
1st Independent Variable	2nd Independent Variable			1st Independent Variable	2nd Independent Variable	Interpolated/ Truncated Value
	25	50	75	0	20	7.02000
0.0011999	7.02	7.02	7.02	0	80	7.02000
0.0012	6.78	6.86	7.02	1.1	20	7.05000
0.01	6.986	6.95	7.02	1.1	80	7.19000
0.1	7.11	7.03	6.97	0.2	20	7.14000
0.5	7.23	7.18	7.14	0.2	80	7.01250
0.9	7.09	7.22	7.18	0	65	7.02000

1	7.05	7.22	7.19	1.1	65	7.20200
				0.25	45	7.10000
				Intermediate Values For Last Data Set		
				7.15500	7.08625	

3.3.9 Input File Used To Test PREWAP Program

line 1 test file

line 2
line 3
Time (yr), Waste Pack Temp.(C), Drip shield temp. (C), Drift wall temp.(C), Invert temp. (C), Waste pack RH, Drip shield RH, Drift wall RH, Backfill RH, Invert RH, Liquid Satr. @ Drip Shield, Liquid Satr.@Invert, Air mass Frac, Water Vapor flux at Dwall (kg/yr/m of drift), Air flux at Dwall(kg/yr/m of drift), A Drip Shield Evapo. rate (m3/yr), Backfill Evapo. Rate (m3/yr), Invert Evapo. Rate (m3/yr), Percolation Flux at 5 m (mm/yr), Vol ume flow at top dripshield (m3/yr), volume flow at invert (m3/yr), Top of the dripshield Temp (C)
The number of Rows = 21
The fraction of this history = 0.000576
line 7
line 8
line 9
line 10
line 11 wpT dsT dwT iT wpRH dsRH dwRH
dsEvapRate pf-5m
0.00 0.222933E+02 -0.999000E+02 0.222797E+02 0.223071E+02 0.999137E+00 -
0.999000E+02 0.999952E+00 -0.999000E+02 0.999180E+00 -0.999000E+02 0.000000E+00 -
0.999000E+02 0.000000E+00 0.000000E+00 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.153137E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
1.00 0.846557E+02 -0.999000E+02 0.679710E+02 0.750104E+02 -0.999000E+02
0.500429E+00 0.999958E+00 -0.999000E+02 0.876529E+00 -0.999000E+02 0.196320E-01 -
0.999000E+02 0.243105E+02 0.106586E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143936E+02 -0.999000E+02 -0.116894E-01 -0.999000E+02
50.00 0.665731E+02 -0.999000E+02 0.612045E+02 0.633398E+02 0.100000E-01 -
0.999000E+02 0.999504E+00 -0.999000E+02 0.967314E+00 -0.999000E+02 0.316090E-01 -
0.999000E+02 0.624383E+01 0.291981E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.142088E+02 -0.999000E+02 -0.279873E-02 -0.999000E+02
50.20 0.236173E+03 0.230511E+03 0.109784E+03 0.188458E+03 0.100000E-01 0.840750E-
01 0.655213E+00 0.969566E+00 0.829800E-01 0.000000E+00 0.000000E+00 0.208500E-02
0.293924E+04 0.834146E+00 -0.123300E-05 0.235282E-02 -0.821340E-04 0.141540E+02
0.000000E+00 0.000000E+00 0.231596E+03
51.00 0.270679E+03 0.266027E+03 0.130378E+03 0.229314E+03 0.100000E-01 0.369300E-
01 0.499133E+00 0.646741E+00 0.347820E-01 0.000000E+00 0.000000E+00 0.792600E-02
0.386056E+02 -0.176730E-01 0.300000E-08 -0.700000E-08 0.170000E-06 0.144618E+02
0.000000E+00 0.000000E+00 0.266970E+03
53.00 0.271006E+03 0.266812E+03 0.143359E+03 0.239704E+03 0.600000E+00 0.298220E-
01 0.365954E+00 0.489141E+00 0.281430E-01 0.000000E+00 0.000000E+00 0.145170E-01
0.102893E+02 0.420108E+00 -0.310800E-05 -0.550000E-07 0.522000E-06 0.150733E+02
0.000000E+00 0.000000E+00 0.267646E+03
55.00 0.261421E+03 0.257416E+03 0.144179E+03 0.240140E+03 0.600000E+00 0.308210E-
01 0.359387E+00 0.480840E+00 0.278820E-01 0.000000E+00 0.000000E+00 0.148380E-01

0.103388E+02 0.472702E+00 -0.355400E-05 -0.580000E-07 0.488000E-06 0.160079E+02
0.000000E+00 0.000000E+00 0.258208E+03
60.00 0.225009E+03 0.221233E+03 0.132806E+03 0.194677E+03 0.600000E+00 0.352420E-01 0.365349E+00 0.491466E+00 0.607210E-01 0.000000E+00 0.000000E+00 0.105486E+00
0.291557E+00 -0.355520E+00 -0.700000E-08 -0.200000E-08 0.390000E-07 0.179075E+02
0.000000E+00 0.000000E+00 0.221968E+03
65.00 0.197084E+03 0.193435E+03 0.120758E+03 0.173413E+03 0.600000E+00 0.535270E-01 0.501935E+00 0.674298E+00 0.954170E-01 0.000000E+00 0.000000E+00 0.130878E+00
0.717410E+00 -0.453557E+00 -0.100000E-08 0.100000E-08 -0.500000E-08 0.216911E+02
0.000000E+00 0.000000E+00 0.194135E+03
70.00 0.144995E+03 0.141441E+03 0.975721E+02 0.128478E+03 0.100000E-01 0.866760E-01 0.748124E+00 0.990652E+00 0.290811E+00 0.000000E+00 0.000000E+00 0.189501E+00
0.265674E+03 0.349618E+02 -0.102500E-05 -0.286851E-02 -0.755000E-06 0.268478E+02
0.000000E+00 0.000000E+00 0.142113E+03
80.00 0.949581E+02 0.915515E+02 0.814937E+02 0.938274E+02 0.600000E+00
0.130910E+00 0.992015E+00 0.997802E+00 0.926671E+00 0.126481E+00 0.609780E-01
0.223147E+00 0.220814E+03 0.193291E+02 0.128079E+00 -0.525328E-02 0.281983E+00
0.275514E+02 0.000000E+00 0.000000E+00 0.921773E+02
100.00 0.900955E+02 0.869274E+02 0.771852E+02 0.899821E+02 0.100000E-01
0.158592E+00 0.994236E+00 0.999768E+00 0.981316E+00 0.161142E+00 0.110698E+00
0.325127E+00 0.128401E+03 0.167901E+02 0.993992E-01 -0.412338E-02 0.248594E+00
0.189149E+02 0.000000E+00 0.000000E+00 0.874805E+02
110.00 0.867760E+02 0.836941E+02 0.745860E+02 0.874209E+02 0.600000E+00
0.170195E+00 0.995199E+00 0.999764E+00 0.984132E+00 0.164643E+00 0.118413E+00
0.395588E+00 0.925944E+02 0.149763E+02 0.861841E-01 -0.368624E-02 0.210613E+00
0.172476E+02 0.000000E+00 0.000000E+00 0.842257E+02
120.00 0.825661E+02 0.795754E+02 0.712272E+02 0.838059E+02 0.100000E-01
0.190156E+00 0.997187E+00 0.999758E+00 0.987154E+00 0.167614E+00 0.122490E+00
0.484554E+00 0.622246E+02 0.125183E+02 0.700028E-01 -0.307191E-02 0.169845E+00
0.162730E+02 0.000000E+00 0.000000E+00 0.800842E+02
130.00 0.810327E+02 0.781357E+02 0.700483E+02 0.824621E+02 0.100000E-01
0.219832E+00 0.998197E+00 0.999755E+00 0.988637E+00 0.168528E+00 0.123351E+00
0.514527E+00 0.543765E+02 0.116858E+02 0.647288E-01 -0.262423E-02 0.156327E+00
0.155837E+02 0.000000E+00 0.000000E+00 0.786208E+02
140.00 0.776294E+02 0.748289E+02 0.675343E+02 0.794910E+02 0.600000E+00
0.247555E+00 0.999252E+00 0.999748E+00 0.991091E+00 0.170812E+00 0.125106E+00
0.576015E+00 0.410952E+02 0.998433E+01 0.538530E-01 -0.230470E-02 0.129704E+00
0.150984E+02 0.000000E+00 0.000000E+00 0.752897E+02
150.00 0.737673E+02 0.710678E+02 0.647680E+02 0.761593E+02 0.600000E+00
0.279064E+00 0.999473E+00 0.999745E+00 0.993142E+00 0.183805E+00 0.136964E+00
0.637418E+00 0.301292E+02 0.797134E+01 0.432977E-01 -0.192148E-02 0.104080E+00
0.147780E+02 0.000000E+00 0.000000E+00 0.715033E+02
190.00 0.712332E+02 0.687596E+02 0.629677E+02 0.739267E+02 0.100000E-01
0.343920E+00 0.999606E+00 0.999741E+00 0.993787E+00 0.186603E+00 0.139378E+00
0.674327E+00 0.247632E+02 0.682169E+01 0.372664E-01 -0.176730E-02 0.896966E-01
0.143423E+02 0.000000E+00 0.000000E+00 0.691465E+02
270.00 0.690627E+02 0.668984E+02 0.613302E+02 0.718319E+02 0.100000E-01
0.442273E+00 0.999772E+00 0.999737E+00 0.994472E+00 0.187777E+00 0.140144E+00
0.705799E+00 0.207220E+02 0.593611E+01 0.322745E-01 -0.153458E-02 0.776633E-01
0.139374E+02 0.118268E+00 -0.358887E-01 0.672245E+02
615.00 0.671101E+02 0.656206E+02 0.596731E+02 0.696723E+02 0.100000E-01
0.673121E+00 0.999966E+00 0.999733E+00 0.996401E+00 0.188846E+00 0.140840E+00
0.735027E+00 0.172995E+02 0.511785E+01 0.276815E-01 -0.114842E-02 0.662257E-01
0.145990E+02 0.398767E-01 -0.350144E-01 0.658302E+02
1000000.00 0.187600E+02 0.187354E+02 0.186076E+02 0.187464E+02 0.998407E+00
0.999883E+00 0.999964E+00 0.999686E+00 0.999958E+00 0.224044E+00 0.166789E+00

0.984671E+00 0.132790E-01 -0.110600E-02 0.268370E-04 -0.663300E-05 0.548690E-04
0.610027E+02 0.112866E-02 0.184060E+00 0.187314E+02
The number of Rows = 29
The fraction of this history = 0.000960
line 3
″
line 4
line 5
line 6
line 7 wpT dsT dwT iT wpRH dsRH dwRH
dsEvapRate pf-5m
″
0.00 0.223001E+02 -0.999000E+02 0.222865E+02 0.223136E+02 0.999138E+00 -
0.999000E+02 0.999952E+00 -0.999000E+02 0.999180E+00 -0.999000E+02 0.000000E+00 -
0.999000E+02 0.000000E+00 0.000000E+00 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.152617E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
1.00 0.806202E+02 -0.999000E+02 0.633204E+02 0.707888E+02 0.477524E+00 -
0.999000E+02 0.999955E+00 -0.999000E+02 0.886023E+00 -0.999000E+02 0.190470E-01 -
0.999000E+02 0.224813E+02 0.119247E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143430E+02 -0.999000E+02 -0.116604E-01 -0.999000E+02
2.00 0.874782E+02 -0.999000E+02 0.717236E+02 0.784255E+02 0.527047E+00 -
0.999000E+02 0.999416E+00 -0.999000E+02 0.869311E+00 -0.999000E+02 0.182770E-01 -
0.999000E+02 0.259342E+02 0.102259E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143530E+02 -0.999000E+02 -0.725051E-02 -0.999000E+02
5.00 0.944264E+02 -0.999000E+02 0.808013E+02 0.866099E+02 0.589066E+00 -
0.999000E+02 0.996760E+00 -0.999000E+02 0.856647E+00 -0.999000E+02 0.963900E-02 -
0.999000E+02 0.304570E+02 0.102450E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144701E+02 -0.999000E+02 -0.117121E-02 -0.999000E+02
20.00 0.890934E+02 -0.999000E+02 0.797213E+02 0.834106E+02 0.688934E+00 -
0.999000E+02 0.995898E+00 -0.999000E+02 0.900721E+00 -0.999000E+02 0.282600E-02 -
0.999000E+02 0.171358E+02 0.707731E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.145367E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
25.00 0.852817E+02 -0.999000E+02 0.767855E+02 0.801724E+02 0.707787E+00 -
0.999000E+02 0.996314E+00 -0.999000E+02 0.912235E+00 -0.999000E+02 0.982700E-02 -
0.999000E+02 0.144370E+02 0.576231E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144728E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
30.00 0.817664E+02 -0.999000E+02 0.740034E+02 0.771318E+02 0.724692E+00 -
0.999000E+02 0.996711E+00 -0.999000E+02 0.925986E+00 -0.999000E+02 0.132880E-01 -
0.999000E+02 0.127767E+02 0.525119E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144009E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
40.00 0.749153E+02 -0.999000E+02 0.684373E+02 0.710976E+02 0.756514E+00 -
0.999000E+02 0.997577E+00 -0.999000E+02 0.946729E+00 -0.999000E+02 0.171170E-01 -
0.999000E+02 0.971942E+01 0.456280E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.142671E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
50.00 0.678115E+02 -0.999000E+02 0.625164E+02 0.647416E+02 0.788405E+00 -
0.999000E+02 0.999037E+00 -0.999000E+02 0.963607E+00 -0.999000E+02 0.284150E-01 -
0.999000E+02 0.707103E+01 0.310949E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.141580E+02 -0.999000E+02 -0.278996E-02 -0.999000E+02
50.20 0.234737E+03 0.229075E+03 0.109300E+03 0.187167E+03 0.762630E-01 0.100000E-
01 0.658942E+00 0.980873E+00 0.847710E-01 0.000000E+00 0.000000E+00 0.203100E-02
0.303839E+04 0.855563E+00 -0.129200E-05 0.307937E-02 -0.861920E-04 0.141030E+02
0.000000E+00 0.000000E+00 0.230161E+03
51.00 0.268555E+03 0.263902E+03 0.127610E+03 0.226167E+03 0.362760E-01 0.100000E-
01 0.527864E+00 0.680440E+00 0.370450E-01 0.000000E+00 0.000000E+00 0.643000E-02
0.128020E+03 -0.416400E-02 0.200000E-08 0.400000E-08 0.193000E-06 0.144098E+02
0.000000E+00 0.000000E+00 0.264845E+03

53.00 0.274117E+03 0.269923E+03 0.142879E+03 0.239454E+03 0.282400E-01 0.100000E-01 0.369748E+00 0.493922E+00 0.282940E-01 0.000000E+00 0.000000E+00 0.143340E-01 0.102595E+02 0.386741E+00 -0.283100E-05 -0.520000E-07 0.542000E-06 0.150223E+02 0.000000E+00 0.000000E+00 0.270758E+03
55.00 0.265761E+03 0.261756E+03 0.144988E+03 0.240575E+03 0.283890E-01 0.600000E+00 0.352861E+00 0.472570E+00 0.276230E-01 0.000000E+00 0.000000E+00 0.151570E-01 0.102755E+02 0.521326E+00 -0.397400E-05 -0.620000E-07 0.455000E-06 0.159587E+02 0.000000E+00 0.000000E+00 0.262547E+03
60.00 0.231692E+03 0.227916E+03 0.136306E+03 0.201924E+03 0.308040E-01 0.600000E+00 0.342139E+00 0.460237E+00 0.542150E-01 0.000000E+00 0.000000E+00 0.926510E-01 0.163887E+00 -0.218317E+00 -0.400000E-08 -0.200000E-08 -0.110000E-07 0.178319E+02 0.000000E+00 0.000000E+00 0.228651E+03
65.00 0.198981E+03 0.195333E+03 0.122966E+03 0.177266E+03 0.467120E-01 0.600000E+00 0.473065E+00 0.635232E+00 0.877210E-01 0.000000E+00 0.000000E+00 0.124235E+00 0.474730E+00 -0.461679E+00 -0.100000E-08 0.400000E-08 0.890000E-07 0.215856E+02 0.000000E+00 0.000000E+00 0.196033E+03
70.00 0.139131E+03 0.135577E+03 0.976314E+02 0.128600E+03 0.781570E-01 0.600000E+00 0.746703E+00 0.989340E+00 0.289581E+00 0.000000E+00 0.000000E+00 0.190654E+00 0.265218E+03 0.348544E+02 -0.103400E-05 -0.285501E-02 -0.763000E-06 0.268695E+02 0.000000E+00 0.000000E+00 0.136249E+03
80.00 0.100158E+03 0.967514E+02 0.857046E+02 0.970909E+02 0.115084E+00 0.100000E-01 0.985973E+00 0.995477E+00 0.884019E+00 0.650060E-01 0.264120E-01 0.146113E+00 0.397487E+03 0.303699E+02 0.153011E+00 -0.498900E-02 0.204364E+00 0.275664E+02 0.000000E+00 0.000000E+00 0.973771E+02
100.00 0.934533E+02 0.902852E+02 0.818526E+02 0.942050E+02 0.140307E+00 0.600000E+00 0.990235E+00 0.997121E+00 0.919350E+00 0.124630E+00 0.604280E-01 0.217854E+00 0.229181E+03 0.193812E+02 0.130214E+00 -0.515831E-02 0.235767E+00 0.188267E+02 0.000000E+00 0.000000E+00 0.908383E+02
110.00 0.887102E+02 0.856283E+02 0.795500E+02 0.922187E+02 0.150632E+00 0.100000E-01 0.991787E+00 0.999695E+00 0.959159E+00 0.141891E+00 0.773060E-01 0.267986E+00 0.172739E+03 0.181566E+02 0.112748E+00 -0.293494E-02 0.271712E+00 0.171724E+02 0.000000E+00 0.000000E+00 0.861599E+02
120.00 0.874543E+02 0.844636E+02 0.784762E+02 0.912332E+02 0.168459E+00 0.600000E+00 0.992456E+00 0.999765E+00 0.975882E+00 0.151229E+00 0.917010E-01 0.293625E+00 0.151039E+03 0.175141E+02 0.105458E+00 -0.453336E-02 0.266612E+00 0.162056E+02 0.000000E+00 0.000000E+00 0.849724E+02
130.00 0.840941E+02 0.811971E+02 0.756464E+02 0.885412E+02 0.194897E+00 0.100000E-01 0.993634E+00 0.999763E+00 0.980092E+00 0.162964E+00 0.115489E+00 0.368973E+00 0.104537E+03 0.155809E+02 0.912377E-01 -0.373414E-02 0.225596E+00 0.155216E+02 0.000000E+00 0.000000E+00 0.816822E+02
140.00 0.807761E+02 0.779757E+02 0.729943E+02 0.857868E+02 0.220070E+00 0.100000E-01 0.995169E+00 0.999759E+00 0.982636E+00 0.165588E+00 0.120302E+00 0.439992E+00 0.758019E+02 0.136974E+02 0.778465E-01 -0.346009E-02 0.190273E+00 0.150399E+02 0.000000E+00 0.000000E+00 0.784364E+02
150.00 0.777314E+02 0.750318E+02 0.706811E+02 0.832177E+02 0.248718E+00 0.600000E+00 0.997062E+00 0.999755E+00 0.985363E+00 0.167470E+00 0.122409E+00 0.499941E+00 0.580119E+02 0.120507E+02 0.671403E-01 -0.294301E-02 0.162715E+00 0.147219E+02 0.000000E+00 0.000000E+00 0.754674E+02
180.00 0.752735E+02 0.727402E+02 0.687718E+02 0.809819E+02 0.293681E+00 0.600000E+00 0.999266E+00 0.999751E+00 0.988900E+00 0.168870E+00 0.123639E+00 0.546981E+00 0.468024E+02 0.107262E+02 0.588192E-01 -0.261450E-02 0.142453E+00 0.143975E+02 0.000000E+00 0.000000E+00 0.731398E+02
225.00 0.729992E+02 0.706785E+02 0.668359E+02 0.786637E+02 0.355414E+00 0.100000E-01 0.998974E+00 0.999745E+00 0.989652E+00 0.171033E+00 0.125191E+00 0.593248E+00 0.378513E+02 0.950032E+01 0.507596E-01 -0.230120E-02 0.122659E+00 0.140623E+02 0.000000E+00 0.000000E+00 0.710345E+02

315.00 0.707678E+02 0.687327E+02 0.649136E+02 0.763492E+02 0.442330E+00
0.100000E-01 0.999309E+00 0.999745E+00 0.991455E+00 0.182473E+00 0.135905E+00
0.635019E+00 0.304144E+02 0.802757E+01 0.435520E-01 -0.194807E-02 0.104876E+00
0.138135E+02 0.968528E-01 -0.127453E+00 0.690353E+02
475.00 0.686313E+02 0.669335E+02 0.628589E+02 0.737972E+02 0.548132E+00
0.100000E-01 0.999531E+00 0.999740E+00 0.992464E+00 0.185740E+00 0.138739E+00
0.677026E+00 0.243129E+02 0.672385E+01 0.366556E-01 -0.170702E-02 0.881237E-01
0.137836E+02 0.574295E-01 -0.773144E-01 0.671779E+02
615.00 0.671560E+02 0.656666E+02 0.614066E+02 0.719363E+02 0.630850E+00
0.600000E+00 0.999704E+00 0.999736E+00 0.993185E+00 0.186764E+00 0.139402E+00
0.704846E+00 0.207516E+02 0.593717E+01 0.323022E-01 -0.150387E-02 0.778167E-01
0.145462E+02 0.396563E-01 -0.347207E-01 0.658761E+02
1000000.00 0.188336E+02 0.188090E+02 0.186851E+02 0.188401E+02 0.998413E+00
0.999883E+00 0.999964E+00 0.999686E+00 0.999958E+00 0.223843E+00 0.166600E+00
0.984575E+00 0.151070E-01 -0.179900E-02 0.296850E-04 -0.676300E-05 0.632210E-04
0.607919E+02 0.112650E-02 0.183561E+00 0.188050E+02
The number of Rows = 32
The fraction of this history = 0.001153
Coordinate Location:
The easting coordinate = 170256.20 m
The northing coordinate = 234314.20 m
Infiltration rate:
qinf = 60.37322 mm/yr
0 2.23E+01 -9.99E+01 2.23E+01 2.23E+01 9.99E-01 -9.99E+01 1.00E+00 -9.99E+01
9.99E-01 -9.99E+01 0.00E+00 -9.99E+01 0.00E+00 0.00E+00 -9.99E+01 -9.99E+01 -
9.99E+01 1.52E+01 -9.99E+01 0.00E+00 -9.99E+01
″
1 7.88E+01 -9.99E+01 6.12E+01 6.88E+01 4.67E-01 -9.99E+01 1.00E+00 -9.99E+01
8.90E-01 -9.99E+01 1.86E-02 -9.99E+01 2.15E+01 1.24E+01 -9.99E+01 -9.99E+01 -
9.99E+01 1.42E+01 -9.99E+01 -1.16E-02 -9.99E+01
″
40 7.56E+01 -9.99E+01 6.91E+01 7.19E+01 7.56E-01 -9.99E+01 9.97E-01 -9.99E+01
9.43E-01 -9.99E+01 1.66E-02 -9.99E+01 1.00E+01 4.62E+00 -9.99E+01 -9.99E+01 -
9.99E+01 1.42E+01 -9.99E+01 0.00E+00 -9.99E+01
″
50.2 2.26E+02 2.20E+02 1.06E+02 1.82E+02 4.90E-01 5.50E-01 6.78E-01 1.00E+00
9.38E-02 0.00E+00 0.00E+00 4.08E-02 2.91E+03 4.62E+00 -1.25E-06 6.81E-03 -
8.42E-05 1.40E+01 0.00E+00 0.00E+00 2.21E+02
″
51 2.64E+02 2.60E+02 1.23E+02 2.20E+02 5.50E-01 6.50E-01 5.56E-01 7.18E-01
4.24E-02 0.00E+00 0.00E+00 4.70E-03 5.85E+02 1.78E-01 -5.00E-09 2.50E-08
1.26E-06 1.43E+01 0.00E+00 0.00E+00 2.61E+02
″
52 2.74E+02 2.69E+02 1.34E+02 2.33E+02 6.50E-01 8.50E-01 4.54E-01 5.95E-01
3.23E-02 0.00E+00 0.00E+00 1.02E-02 2.39E+01 1.90E-02 0.00E+00 -1.80E-08
4.61E-07 1.46E+01 0.00E+00 0.00E+00 2.70E+02
″
55 2.72E+02 2.68E+02 1.45E+02 2.40E+02 8.50E-01 4.90E-01 3.55E-01 4.76E-01
2.77E-02 0.00E+00 0.00E+00 1.50E-02 1.01E+01 4.94E-01 -3.75E-06 -6.00E-08
4.68E-07 1.59E+01 0.00E+00 0.00E+00 2.69E+02
″
60 2.55E+02 2.51E+02 1.45E+02 2.19E+02 9.00E-01 9.50E-01 2.87E-01 3.87E-01
3.88E-02 0.00E+00 0.00E+00 6.17E-02 -1.31E-01 9.90E-02 3.00E-09 -3.00E-09 -
1.03E-07 1.96E+01 0.00E+00 0.00E+00 2.52E+02
″

65 2.26E+02 2.22E+02 1.35E+02 2.00E+02 9.50E-01 9.00E-01 3.48E-01 4.68E-01
5.60E-02 0.00E+00 0.00E+00 9.70E-02 1.96E-01 -2.53E-01 -4.00E-09 -2.00E-09 -
8.00E-09 2.14E+01 0.00E+00 0.00E+00 2.23E+02
"

1180 6.54E+01 6.44E+01 6.01E+01 7.02E+01 4.90E-01 5.50E-01 1.00E+00 1.00E+00
9.94E-01 1.86E-01 1.39E-01 7.29E-01 1.77E+01 5.21E+00 2.83E-02 -1.14E-03
6.87E-02 3.91E+01 1.35E-02 9.16E-02 6.46E+01
"

1420 6.34E+01 6.25E+01 5.80E+01 6.75E+01 5.50E-01 6.50E-01 1.00E+00 1.00E+00
9.98E-01 1.87E-01 1.41E-01 7.63E-01 1.42E+01 4.33E+00 2.31E-02 -9.44E-04
5.61E-02 3.93E+01 9.53E-03 1.01E-01 6.26E+01
"

1680 6.13E+01 6.05E+01 5.60E+01 6.48E+01 6.50E-01 8.50E-01 1.00E+00 1.00E+00
9.99E-01 1.89E-01 1.43E-01 7.92E-01 1.14E+01 3.59E+00 1.90E-02 -7.95E-04
4.71E-02 3.94E+01 7.26E-03 1.06E-01 6.06E+01
"

1900 5.94E+01 5.86E+01 5.41E+01 6.22E+01 8.50E-01 4.90E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.17E-01 9.15E+00 2.97E+00 1.55E-02 -7.74E-04
3.84E-02 3.96E+01 5.85E-03 1.10E-01 5.87E+01
"

1950 5.91E+01 5.84E+01 5.38E+01 6.19E+01 9.00E-01 9.50E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.20E-01 8.90E+00 2.89E+00 1.51E-02 -7.60E-04
3.75E-02 4.14E+01 5.80E-03 1.16E-01 5.85E+01
"

1975 5.90E+01 5.83E+01 5.37E+01 6.17E+01 9.50E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.21E-01 8.79E+00 2.86E+00 1.49E-02 -7.54E-04
3.71E-02 4.32E+01 5.81E-03 1.21E-01 5.84E+01
"

2060 5.89E+01 5.82E+01 5.36E+01 6.16E+01 4.90E-01 5.50E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.23E-01 8.69E+00 2.83E+00 1.48E-02 -7.48E-04
3.67E-02 4.50E+01 5.83E-03 1.26E-01 5.83E+01
"

2080 5.88E+01 5.81E+01 5.35E+01 6.14E+01 5.50E-01 6.50E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.24E-01 8.58E+00 2.80E+00 1.46E-02 -7.43E-04
3.63E-02 4.67E+01 5.84E-03 1.32E-01 5.82E+01
"

2100 5.87E+01 5.80E+01 5.34E+01 6.13E+01 6.50E-01 8.50E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.25E-01 8.48E+00 2.77E+00 1.44E-02 -7.37E-04
3.59E-02 4.85E+01 5.86E-03 1.37E-01 5.81E+01
"

2120 5.86E+01 5.79E+01 5.33E+01 6.12E+01 8.50E-01 4.90E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.26E-01 8.38E+00 2.75E+00 1.43E-02 -7.31E-04
3.56E-02 5.03E+01 5.87E-03 1.42E-01 5.80E+01
"

2140 2.00E+01 5.78E+01 5.32E+01 6.10E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.28E-01 8.28E+00 2.72E+00 1.00E+00 -7.26E-04
3.52E-02 1.00E+00 5.89E-03 1.48E-01 5.79E+01
"

2160 2.00E+01 5.77E+01 5.31E+01 6.09E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.29E-01 8.18E+00 2.69E+00 4.50E-01 -7.21E-04
3.48E-02 1.00E+00 5.90E-03 1.53E-01 5.78E+01
"

2180 2.00E+01 5.76E+01 5.30E+01 6.08E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.30E-01 8.09E+00 2.66E+00 0.00E+00 -7.05E-04
3.45E-02 1.00E+00 5.92E-03 1.58E-01 5.77E+01
"

2200 2.00E+01 5.75E+01 5.29E+01 6.06E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.31E-01 8.01E+00 2.62E+00 -1.00E-02 -6.83E-04
3.41E-02 1.00E+00 5.93E-03 1.64E-01 5.76E+01
″
2600 4.40E+01 5.57E+01 5.12E+01 5.82E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.96E-01 1.46E-01 8.51E-01 6.41E+00 2.10E+00 1.00E+00 -4.56E-04
2.76E-02 1.00E+00 4.99E-03 1.69E-01 5.58E+01
″
3050 5.60E+01 5.40E+01 4.95E+01 5.61E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.98E-01 1.47E-01 8.67E-01 5.34E+00 1.78E+00 4.50E-01 -4.21E-04
2.33E-02 1.00E+00 4.46E-03 1.72E-01 5.41E+01
″
3600 6.70E+01 5.24E+01 4.80E+01 5.40E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.99E-01 1.47E-01 8.81E-01 4.45E+00 1.48E+00 0.00E+00 -3.67E-04
1.96E-02 1.00E+00 3.96E-03 1.73E-01 5.24E+01
″
4300 6.70E+01 5.06E+01 4.63E+01 5.18E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 2.00E-01 1.48E-01 8.94E-01 3.57E+00 1.22E+00 -1.00E-02 -3.94E-04
1.61E-02 1.00E+00 3.84E-03 1.74E-01 5.07E+01
″
5100 9.80E+01 4.89E+01 4.48E+01 5.00E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 2.06E-01 1.54E-01 9.04E-01 3.08E+00 9.34E-01 1.00E+00 -2.72E-04
1.39E-02 1.00E+00 3.44E-03 1.75E-01 4.90E+01
″
6000 9.80E+01 4.73E+01 4.33E+01 4.81E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 2.08E-01 1.55E-01 9.13E-01 2.61E+00 7.93E-01 4.50E-01 -2.42E-04
1.17E-02 1.00E+00 3.02E-03 1.88E-01 4.73E+01
″
7000 9.80E+01 4.56E+01 4.17E+01 4.64E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 2.09E-01 1.56E-01 9.21E-01 2.27E+00 7.00E-01 0.00E+00 -2.02E-04
1.02E-02 1.00E+00 2.90E-03 2.05E-01 4.57E+01
″
8000 9.80E+01 4.42E+01 4.04E+01 4.48E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 2.10E-01 1.56E-01 9.27E-01 2.00E+00 6.17E-01 -1.00E-02 -1.74E-04
9.11E-03 1.00E+00 2.64E-03 2.19E-01 4.42E+01
″
1000000 1.89E+01 1.89E+01 1.88E+01 1.89E+01 9.00E-01 9.00E-01 1.00E+00
1.00E+00 1.00E+00 2.24E-01 1.66E-01 9.84E-01 1.66E-02 -5.50E-03 3.20E-05 -
6.84E-06 7.01E-05 6.04E+01 1.12E-03 2.21E-01 1.89E+01

3.3.10 Output From PREWAP Test Case

! 1st comment line
! 2nd comment line
! 3rd comment line
3 21
17
5.760E-04
! t wpT wpRH dsT dsRH wpPHnd wpCLnd wpPHd wpCLd
dsPHnd dsCLnd dsPHd dsCLd ipkPHnd ipkCLnd ipkPHd ipkCLd barPHnd
barCLnd barPHd barCLd PercFlux5m

5.100E+01 2.707E+02 1.000E-02 2.660E+02 3.693E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.446E+01
5.300E+01 2.710E+02 6.000E-01 2.668E+02 2.982E-02 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.507E+01
5.500E+01 2.614E+02 6.000E-01 2.574E+02 3.082E-02 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.601E+01
6.000E+01 2.250E+02 6.000E-01 2.212E+02 3.524E-02 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.791E+01
6.500E+01 1.971E+02 6.000E-01 1.934E+02 5.353E-02 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.169E+01
7.000E+01 1.450E+02 1.000E-02 1.414E+02 8.668E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.685E+01
8.000E+01 9.496E+01 6.000E-01 9.155E+01 1.309E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.755E+01
1.000E+02 9.010E+01 1.000E-02 8.693E+01 1.586E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.891E+01
1.100E+02 8.678E+01 6.000E-01 8.369E+01 1.702E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.725E+01
1.200E+02 8.257E+01 1.000E-02 7.958E+01 1.902E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.627E+01
1.300E+02 8.103E+01 1.000E-02 7.814E+01 2.198E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.558E+01
1.400E+02 7.763E+01 6.000E-01 7.483E+01 2.476E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.510E+01
1.500E+02 7.377E+01 6.000E-01 7.107E+01 2.791E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.478E+01
1.900E+02 7.123E+01 1.000E-02 6.876E+01 3.439E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.434E+01
2.700E+02 6.906E+01 1.000E-02 6.690E+01 4.423E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.394E+01
6.150E+02 6.711E+01 1.000E-02 6.562E+01 6.731E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.460E+01
1.000E+06 1.876E+01 9.984E-01 1.874E+01 9.999E-01 -9.990E-02 9.980E-03 7.188E+00
5.166E+01 -9.990E-02 9.980E-03 7.188E+00 5.166E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 6.100E+01
19
9.600E-04
! t wpT wpRH dsT dsRH wpPHnd wpCLnd wpPHd wpCLd
dsPHnd dsCLnd dsPHd dsCLd ipkPHnd ipkCLnd ipkPHd ipkCLd barPHnd
barCLnd barPHd barCLd PercFlux5m

5.020E+01 2.347E+02 7.626E-02 2.291E+02 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.410E+01
5.300E+01 2.741E+02 2.824E-02 2.699E+02 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.502E+01
5.500E+01 2.658E+02 2.839E-02 2.618E+02 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.596E+01
6.000E+01 2.317E+02 3.080E-02 2.279E+02 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.783E+01
6.500E+01 1.990E+02 4.671E-02 1.953E+02 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.159E+01
7.000E+01 1.391E+02 7.816E-02 1.356E+02 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.687E+01
8.000E+01 1.002E+02 1.151E-01 9.675E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.757E+01
1.000E+02 9.345E+01 1.403E-01 9.029E+01 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.883E+01
1.100E+02 8.871E+01 1.506E-01 8.563E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.717E+01
1.200E+02 8.745E+01 1.685E-01 8.446E+01 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.621E+01
1.300E+02 8.409E+01 1.949E-01 8.120E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.552E+01
1.400E+02 8.078E+01 2.201E-01 7.798E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.504E+01
1.500E+02 7.773E+01 2.487E-01 7.503E+01 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.472E+01
1.800E+02 7.527E+01 2.937E-01 7.274E+01 6.000E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.440E+01
2.250E+02 7.300E+01 3.554E-01 7.068E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.406E+01
3.150E+02 7.077E+01 4.423E-01 6.873E+01 1.000E-02 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.381E+01
4.750E+02 6.863E+01 5.481E-01 6.693E+01 1.000E-02 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.378E+01
6.150E+02 6.716E+01 6.309E-01 6.567E+01 6.000E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.455E+01

1.000E+06 1.883E+01 9.984E-01 1.881E+01 9.999E-01 -9.990E-02 9.980E-03 7.187E+00
5.166E+01 -9.990E-02 9.980E-03 7.187E+00 5.166E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 6.079E+01
29
1.153E-03
! t wpT wpRH dsT dsRH wpPHnd wpCLnd wpPHd wpCLd
dsPHnd dsCLnd dsPHd dsCLd ipkPHnd ipkCLnd ipkPHd ipkCLd barPHnd
barCLnd barPHd barCLd PercFlux5m
5.020E+01 2.260E+02 4.900E-01 2.200E+02 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.400E+01
5.100E+01 2.640E+02 5.500E-01 2.600E+02 6.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.430E+01
5.200E+01 2.740E+02 6.500E-01 2.690E+02 8.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.460E+01
5.500E+01 2.720E+02 8.500E-01 2.680E+02 4.900E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.590E+01
6.000E+01 2.550E+02 9.000E-01 2.510E+02 9.500E-01 -9.990E-02 9.980E-03 8.580E+00
7.362E+01 -9.990E-02 9.980E-03 8.580E+00 7.362E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.960E+01
6.500E+01 2.260E+02 9.500E-01 2.220E+02 9.000E-01 -9.990E-02 9.980E-03 8.580E+00
7.362E+01 -9.990E-02 9.980E-03 8.580E+00 7.362E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.140E+01
1.180E+03 6.540E+01 4.900E-01 6.440E+01 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.910E+01
1.420E+03 6.340E+01 5.500E-01 6.250E+01 6.500E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.930E+01
1.680E+03 6.130E+01 6.500E-01 6.050E+01 8.500E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.940E+01
1.900E+03 5.940E+01 8.500E-01 5.860E+01 4.900E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.960E+01
1.950E+03 5.910E+01 9.000E-01 5.840E+01 9.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.140E+01
1.975E+03 5.900E+01 9.500E-01 5.830E+01 9.000E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.320E+01
2.060E+03 5.890E+01 4.900E-01 5.820E+01 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.500E+01
2.080E+03 5.880E+01 5.500E-01 5.810E+01 6.500E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.670E+01
2.100E+03 5.870E+01 6.500E-01 5.800E+01 8.500E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.850E+01
2.120E+03 5.860E+01 8.500E-01 5.790E+01 4.900E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 5.030E+01

2.140E+03 2.000E+01 9.000E-01 5.780E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
2.160E+03 2.000E+01 9.000E-01 5.770E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
2.180E+03 2.000E+01 9.000E-01 5.760E+01 9.000E-01 -9.990E-02 9.980E-03 7.190E+00
5.170E+01 -9.990E-02 9.980E-03 7.190E+00 5.170E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
2.200E+03 2.000E+01 9.000E-01 5.750E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
2.600E+03 4.400E+01 9.000E-01 5.570E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
3.050E+03 5.600E+01 9.000E-01 5.400E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
3.600E+03 6.700E+01 9.000E-01 5.240E+01 9.000E-01 -9.990E-02 9.980E-03 7.190E+00
5.170E+01 -9.990E-02 9.980E-03 7.190E+00 5.170E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
4.300E+03 6.700E+01 9.000E-01 5.060E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
5.100E+03 9.800E+01 9.000E-01 4.890E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
6.000E+03 9.800E+01 9.000E-01 4.730E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
7.000E+03 9.800E+01 9.000E-01 4.560E+01 9.000E-01 -9.990E-02 9.980E-03 7.190E+00
5.170E+01 -9.990E-02 9.980E-03 7.190E+00 5.170E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
8.000E+03 9.800E+01 9.000E-01 4.420E+01 9.000E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.000E+00
1.000E+06 1.890E+01 9.000E-01 1.890E+01 9.000E-01 -9.990E-02 9.980E-03 7.187E+00
5.166E+01 -9.990E-02 9.980E-03 7.187E+00 5.166E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 6.040E+01

3.3.11 EXCEL Spreadsheet Replicating PREWAP Test Case

Time Period	Time (yr),	Waste Pack Temp.(C),	Drip shield temp. (C),		Drift wall temp.(C),	Invert temp. (C),	Waste pack RH,	RH	pH	Reason	Drip shield RH,	RH
1st Data Set Page 1												
1st	0.0	22.29	-99.90	dst<0	22.28	22.31	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	84.66	-99.90	dst<0	67.97	75.01	-99.90	-100.40	-0.0999	< 50 Yrs	0.500	0.00
2nd	50.0	66.57	-99.90	dst<0	61.20	63.34	0.01	-0.49	-0.0999	RH<0.5	-99.900	-100.40
2nd	50.2	236.17	230.51		109.78	188.46	0.01	-0.49	-0.0999	RH<0.5	0.084	-0.42
2nd	51.0	270.68	266.03		130.38	229.31	0.01	-0.49	-0.0999	RH<0.5	0.037	-0.46
2nd	53.0	271.01	266.81		143.36	239.70	0.60	0.10	9.4000	pH const	0.030	-0.47
2nd	55.0	261.42	257.42		144.18	240.14	0.60	0.10	9.4000	pH const	0.031	-0.47
2nd	60.0	225.01	221.23		132.81	194.68	0.60	0.10	9.4000	pH const	0.035	-0.47
2nd	65.0	197.08	193.44		120.76	173.41	0.60	0.10	9.4000	pH const	0.054	-0.45
2nd	70.0	145.00	141.44		97.57	128.48	0.01	-0.49	-0.0999	RH<0.5	0.087	-0.41
2nd	80.0	94.96	91.55		81.49	93.83	0.60	0.10	9.4000	pH const	0.131	-0.37
2nd	100.0	90.10	86.93		77.19	89.98	0.01	-0.49	-0.0999	RH<0.5	0.159	-0.34
2nd	110.0	86.78	83.69		74.59	87.42	0.60	0.10	9.4000	pH const	0.170	-0.33
2nd	120.0	82.57	79.58		71.23	83.81	0.01	-0.49	-0.0999	RH<0.5	0.190	-0.31
2nd	130.0	81.03	78.14		70.05	82.46	0.01	-0.49	-0.0999	RH<0.5	0.220	-0.28
2nd	140.0	77.63	74.83		67.53	79.49	0.60	0.10	9.4000	pH const	0.248	-0.25
2nd	150.0	73.77	71.07		64.77	76.16	0.60	0.10	9.4000	pH const	0.279	-0.22
2nd	190.0	71.23	68.76		62.97	73.93	0.01	-0.49	-0.0999	RH<0.5	0.344	-0.16
2nd	270.0	69.06	66.90		61.33	71.83	0.01	-0.49	-0.0999	RH<0.5	0.442	-0.06
2nd	615.0	67.11	65.62		59.67	69.67	0.01	-0.49	-0.0999	RH<0.5	0.673	0.17
	1000000.0	18.76	18.74		18.61	18.75	1.00	0.50		Interpolate	1.000	0.50

Skip if wp or ds Temp < 0	wpRH or dsRH > Cor Lim (.501)	wpRH i<.501 & i+1 >.501	dsRH i<.501 & i+1 >.501	wpRH i<.501 & i-1>=.501	dsRH i<.501 & I-1 >.501	Skip if wpRH I<.501 I+1<.501 , I-1<.501	Skip if dsRH I<.501 I+1<.501 , I-1<.501	SAVE LINE	Drift wall RH,	Backfill RH,	Invert RH,	Liquid Satr. @ Drip Shield,	Liquid Satr.@Invert,	Air mass Frac,
1st Data Set page 2														
TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.88	-99.90	0.02	-99.90
TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	1.00	-99.90	0.97	-99.90	0.03	-99.90
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	0.66	0.97	0.08	0.00	0.00	0.00
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.50	0.65	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.37	0.49	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.36	0.48	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.37	0.49	0.06	0.00	0.00	0.11
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.50	0.67	0.10	0.00	0.00	0.13
FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.75	0.99	0.29	0.00	0.00	0.19
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.99	1.00	0.93	0.13	0.06	0.22
FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.99	1.00	0.98	0.16	0.11	0.33
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.98	0.16	0.12	0.40
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.12	0.48
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.12	0.51
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.13	0.58
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.18	0.14	0.64
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.19	0.14	0.67
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.71
FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.74
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

Water Vapor flux at Dwall (kg/yr/m of drift),	Air flux at Dwall(kg/yr/m of drift),	A Drip Shield Evapo. rate (m3/yr),	Backfill Evapo. Rate (m3/yr),	Invert Evapo. Rate (m3/yr),	Percolation Flux at 5 m (mm/yr),	Volume flow at top dripshield (m3/yr),	volume flow at invert (m3/yr),	Top of the dripshield Temp (C)
1st Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.31	***-99.90***	0.00	-99.90
24.31	10.66	-99.90	-99.90	-99.90	14.39	***-99.90***	-0.01	-99.90
6.24	2.92	-99.90	-99.90	-99.90	14.21	***-99.90***	0.00	-99.90
2939.24	0.83	0.00	0.00	0.00	14.15	0.00	0.00	231.60
38.61	-0.02	0.00	0.00	0.00	14.46	0.00	0.00	266.97
10.29	0.42	0.00	0.00	0.00	15.07	0.00	0.00	267.65
10.34	0.47	0.00	0.00	0.00	16.01	0.00	0.00	258.21
0.29	-0.36	0.00	0.00	0.00	17.91	0.00	0.00	221.97
0.72	-0.45	0.00	0.00	0.00	21.69	0.00	0.00	194.14
265.67	34.96	0.00	0.00	0.00	26.85	0.00	0.00	142.11
220.81	19.33	0.13	-0.01	0.28	27.55	0.00	0.00	92.18
128.40	16.79	0.10	0.00	0.25	18.91	0.00	0.00	87.48
92.59	14.98	0.09	0.00	0.21	17.25	0.00	0.00	84.23
62.22	12.52	0.07	0.00	0.17	16.27	0.00	0.00	80.08
54.38	11.69	0.06	0.00	0.16	15.58	0.00	0.00	78.62
41.10	9.98	0.05	0.00	0.13	15.10	0.00	0.00	75.29
30.13	7.97	0.04	0.00	0.10	14.78	0.00	0.00	71.50
24.76	6.82	0.04	0.00	0.09	14.34	0.00	0.00	69.15
20.72	5.94	0.03	0.00	0.08	13.94	0.12	-0.04	67.22
17.30	5.12	0.03	0.00	0.07	14.60	0.04	-0.04	65.83
0.01	0.00	0.00	0.00	0.00	61.00	0.00	0.18	18.73

2nd Data Set Page 1												
1st	0.0	22.30	-99.90	dst<0	22.29	22.31	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	80.62	-99.90	dst<0	63.32	70.79	0.48	-0.02	-0.0999	< 50 Yrs	-99.900	-100.40
1st	2.0	87.48	-99.90	dst<0	71.72	78.43	0.53	0.03	-0.0999	< 50 Yrs	-99.900	-100.40
1st	5.0	94.43	-99.90	dst<0	80.80	86.61	0.59	0.09	-0.0999	< 50 Yrs	-99.900	-100.40
1st	20.0	89.09	-99.90	dst<0	79.72	83.41	0.69	0.19	-0.0999	< 50 Yrs	-99.900	-100.40
1st	25.0	85.28	-99.90	dst<0	76.79	80.17	0.71	0.21	-0.0999	< 50 Yrs	-99.900	-100.40
1st	30.0	81.77	-99.90	dst<0	74.00	77.13	0.72	0.22	-0.0999	< 50 Yrs	-99.900	-100.40
1st	40.0	74.92	-99.90	dst<0	68.44	71.10	0.76	0.26	-0.0999	< 50 Yrs	-99.900	-100.40
2nd	50.0	67.81	-99.90	dst<0	62.52	64.74	0.79	0.29	-0.0999	Seep< -99	-99.900	-100.40
2nd	50.2	234.74	229.08		109.30	187.17	0.08	-0.42	-0.0999	RH<0.5	0.010	-0.49
2nd	51.0	268.56	263.90		127.61	226.17	0.04	-0.46	-0.0999	RH<0.5	0.010	-0.49
2nd	53.0	274.12	269.92		142.88	239.45	0.03	-0.47	-0.0999	RH<0.5	0.010	-0.49
2nd	55.0	265.76	261.76		144.99	240.58	0.03	-0.47	-0.0999	RH<0.5	0.600	0.10
2nd	60.0	231.69	227.92		136.31	201.92	0.03	-0.47	-0.0999	RH<0.5	0.600	0.10
2nd	65.0	198.98	195.33		122.97	177.27	0.05	-0.45	-0.0999	RH<0.5	0.600	0.10
2nd	70.0	139.13	135.58		97.63	128.60	0.08	-0.42	-0.0999	RH<0.5	0.600	0.10
2nd	80.0	100.16	96.75		85.70	97.09	0.12	-0.39	-0.0999	RH<0.5	0.010	-0.49
2nd	100.0	93.45	90.29		81.85	94.21	0.14	-0.36	-0.0999	RH<0.5	0.600	0.10
2nd	110.0	88.71	85.63		79.55	92.22	0.15	-0.35	-0.0999	RH<0.5	0.010	-0.49
2nd	120.0	87.45	84.46		78.48	91.23	0.17	-0.33	-0.0999	RH<0.5	0.600	0.10
2nd	130.0	84.09	81.20		75.65	88.54	0.19	-0.31	-0.0999	RH<0.5	0.010	-0.49
2nd	140.0	80.78	77.98		72.99	85.79	0.22	-0.28	-0.0999	RH<0.5	0.010	-0.49
2nd	150.0	77.73	75.03		70.68	83.22	0.25	-0.25	-0.0999	RH<0.5	0.600	0.10
2nd	180.0	75.27	72.74		68.77	80.98	0.29	-0.21	-0.0999	RH<0.5	0.600	0.10
2nd	225.0	73.00	70.68		66.84	78.66	0.36	-0.15	-0.0999	RH<0.5	0.010	-0.49
2nd	315.0	70.77	68.73		64.91	76.35	0.44	-0.06	-0.0999	RH<0.5	0.010	-0.49
2nd	475.0	68.63	66.93		62.86	73.80	0.55	0.05	9.4000	pH const	0.010	-0.49
2nd	615.0	67.16	65.67		61.41	71.94	0.63	0.13	9.4000	pH const	0.600	0.10
5th	1000000.0	18.83	18.81		18.69	18.84	1.00	0.50		Interpolate	1.000	0.50

2nd Data Set Page 2														
TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.89	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.87	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.86	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.90	-99.90	0.00	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.91	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.93	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.95	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.96	-99.90	0.03	-99.90
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.66	0.98	0.08	0.00	0.00	0.00
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	0.53	0.68	0.04	0.00	0.00	0.01
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.37	0.49	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.35	0.47	0.03	0.00	0.00	0.02
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.34	0.46	0.05	0.00	0.00	0.09
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.47	0.64	0.09	0.00	0.00	0.12
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.75	0.99	0.29	0.00	0.00	0.19
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.88	0.07	0.03	0.15
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.92	0.12	0.06	0.22
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.96	0.14	0.08	0.27
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.98	0.15	0.09	0.29
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	cull	0.99	1.00	0.98	0.16	0.12	0.37
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.98	0.17	0.12	0.44
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.17	0.12	0.50
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.17	0.12	0.55
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	cull	1.00	1.00	0.99	0.17	0.13	0.59
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.18	0.14	0.64
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.68
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.70
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

2nd Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.26	***-99.90***	0.00	-99.90
22.48	11.92	-99.90	-99.90	-99.90	14.34	***-99.90***	-0.01	-99.90
25.93	10.23	-99.90	-99.90	-99.90	14.35	***-99.90***	-0.01	-99.90
30.46	10.25	-99.90	-99.90	-99.90	14.47	***-99.90***	0.00	-99.90
17.14	7.08	-99.90	-99.90	-99.90	14.54	***-99.90***	0.00	-99.90
14.44	5.76	-99.90	-99.90	-99.90	14.47	***-99.90***	0.00	-99.90
12.78	5.25	-99.90	-99.90	-99.90	14.40	***-99.90***	0.00	-99.90
9.72	4.56	-99.90	-99.90	-99.90	14.27	***-99.90***	0.00	-99.90
7.07	3.11	-99.90	-99.90	-99.90	14.16	***-99.90***	0.00	-99.90
3038.39	0.86	0.00	0.00	0.00	14.10	0.00	0.00	230.16
128.02	0.00	0.00	0.00	0.00	14.41	0.00	0.00	264.85
10.26	0.39	0.00	0.00	0.00	15.02	0.00	0.00	270.76
10.28	0.52	0.00	0.00	0.00	15.96	0.00	0.00	262.55
0.16	-0.22	0.00	0.00	0.00	17.83	0.00	0.00	228.65
0.47	-0.46	0.00	0.00	0.00	21.59	0.00	0.00	196.03
265.22	34.85	0.00	0.00	0.00	26.87	0.00	0.00	136.25
397.49	30.37	0.15	0.00	0.20	27.57	0.00	0.00	97.38
229.18	19.38	0.13	-0.01	0.24	18.83	0.00	0.00	90.84
172.74	18.16	0.11	0.00	0.27	17.17	0.00	0.00	86.16
151.04	17.51	0.11	0.00	0.27	16.21	0.00	0.00	84.97
104.54	15.58	0.09	0.00	0.23	15.52	0.00	0.00	81.68
75.80	13.70	0.08	0.00	0.19	15.04	0.00	0.00	78.44
58.01	12.05	0.07	0.00	0.16	14.72	0.00	0.00	75.47
46.80	10.73	0.06	0.00	0.14	14.40	0.00	0.00	73.14
37.85	9.50	0.05	0.00	0.12	14.06	0.00	0.00	71.03
30.41	8.03	0.04	0.00	0.10	13.81	0.10	-0.13	69.04
24.31	6.72	0.04	0.00	0.09	13.78	0.06	-0.08	67.18
20.75	5.94	0.03	0.00	0.08	14.55	0.04	-0.03	65.88
0.02	0.00	0.00	0.00	0.00	60.79	0.00	0.18	18.81

3rd Data Set Page 1												
1st	0.0	22.30	-99.90	dst<0	22.30	22.30	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	78.80	-99.90	dst<0	61.20	68.80	0.47	-0.03	-0.0999	< 50 Yrs	-99.900	-100.40
1st	40.0	75.60	-99.90	dst<0	69.10	71.90	0.76	0.26	-0.0999	< 50 Yrs	-99.900	-100.40
2nd	50.2	226.00	220.00		106.00	182.00	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
2nd	51.0	264.00	260.00		123.00	220.00	0.55	0.05	9.4000	pH const	0.650	0.15
2nd	52.0	274.00	269.00		134.00	233.00	0.65	0.15	9.4000	pH const	0.850	0.35
2nd	55.0	272.00	268.00		145.00	240.00	0.85	0.35		Interpolate	0.490	-0.01
2nd	60.0	255.00	251.00		145.00	219.00	0.90	0.40		Interpolate	0.950	0.45
2nd	65.0	226.00	222.00		135.00	200.00	0.95	0.45		Interpolate	0.900	0.40
3rd	1180.0	65.40	64.40		60.10	70.20	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
3rd	1420.0	63.40	62.50		58.00	67.50	0.55	0.05	7.6400	pH const	0.650	0.15
3rd	1680.0	61.30	60.50		56.00	64.80	0.65	0.15	7.6400	pH const	0.850	0.35
3rd	1900.0	59.40	58.60		54.10	62.20	0.85	0.35	7.6400	pH const	0.490	-0.01
3rd	1950.0	59.10	58.40		53.80	61.90	0.90	0.40		Interpolate	0.950	0.45
3rd	1975.0	59.00	58.30		53.70	61.70	0.95	0.45		Interpolate	0.900	0.40
4th	2060.0	58.90	58.20		53.60	61.60	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
4th	2080.0	58.80	58.10		53.50	61.40	0.55	0.05	7.0200	pH const	0.650	0.15
4th	2100.0	58.70	58.00		53.40	61.30	0.65	0.15	7.0200	pH const	0.850	0.35
4th	2120.0	58.60	57.90		53.30	61.20	0.85	0.35	7.0200	pH const	0.490	-0.01
4th	2140.0	20.00	57.80		53.20	61.00	0.90	0.40		Interpolate	0.900	0.40
4th	2160.0	20.00	57.70		53.10	60.90	0.90	0.40		Interpolate	0.900	0.40
4th	2180.0	20.00	57.60		53.00	60.80	0.90	0.40		Interpolate	0.900	0.40
4th	2200.0	20.00	57.50		52.90	60.60	0.90	0.40		Interpolate	0.900	0.40
4th	2600.0	44.00	55.70		51.20	58.20	0.90	0.40		Interpolate	0.900	0.40
4th	3050.0	56.00	54.00		49.50	56.10	0.90	0.40		Interpolate	0.900	0.40
4th	3600.0	67.00	52.40		48.00	54.00	0.90	0.40		Interpolate	0.900	0.40
4th	4300.0	67.00	50.60		46.30	51.80	0.90	0.40		Interpolate	0.900	0.40
4th	5100.0	98.00	48.90		44.80	50.00	0.90	0.40		Interpolate	0.900	0.40
4th	6000.0	98.00	47.30		43.30	48.10	0.90	0.40		Interpolate	0.900	0.40
4th	7000.0	98.00	45.60		41.70	46.40	0.90	0.40		Interpolate	0.900	0.40
4th	8000.0	98.00	44.20		40.40	44.80	0.90	0.40		Interpolate	0.900	0.40
5th	1000000.0	18.90	18.90		18.80	18.90	0.90	0.40		Interpolate	0.900	0.40

3rd Data Set Page 2														
TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.89	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	cull	1.00	-99.90	0.94	-99.90	0.02	-99.90
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	0.68	1.00	0.09	0.00	0.00	0.04
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.56	0.72	0.04	0.00	0.00	0.00
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.45	0.60	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	0.36	0.48	0.03	0.00	0.00	0.02
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.29	0.39	0.04	0.00	0.00	0.06
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.35	0.47	0.06	0.00	0.00	0.10
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.73
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.76
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.79
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.85
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.87
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.88
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.89
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.15	0.90
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.91
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.92
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.93
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

3rd Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.20	***-99.90***	0.00	-99.90
21.50	12.40	-99.90	-99.90	-99.90	14.20	***-99.90***	-0.01	-99.90
10.00	4.62	-99.90	-99.90	-99.90	14.20	***-99.90***	0.00	-99.90
2910.00	4.62	0.00	0.01	0.00	14.00	0.00	0.00	221.00
585.00	0.18	0.00	0.00	0.00	14.30	0.00	0.00	261.00
23.90	0.02	0.00	0.00	0.00	14.60	0.00	0.00	270.00
10.10	0.49	0.00	0.00	0.00	15.90	0.00	0.00	269.00
-0.13	0.10	0.00	0.00	0.00	19.60	0.00	0.00	252.00
0.20	-0.25	0.00	0.00	0.00	21.40	0.00	0.00	223.00
17.70	5.21	0.03	0.00	0.07	39.10	0.01	0.09	64.60
14.20	4.33	0.02	0.00	0.06	39.30	0.01	0.10	62.60
11.40	3.59	0.02	0.00	0.05	39.40	0.01	0.11	60.60
9.15	2.97	0.02	0.00	0.04	39.60	0.01	0.11	58.70
8.90	2.89	0.02	0.00	0.04	41.40	0.01	0.12	58.50
8.79	2.86	0.01	0.00	0.04	43.20	0.01	0.12	58.40
8.69	2.83	0.01	0.00	0.04	45.00	0.01	0.13	58.30
8.58	2.80	0.01	0.00	0.04	46.70	0.01	0.13	58.20
8.48	2.77	0.01	0.00	0.04	48.50	0.01	0.14	58.10
8.38	2.75	0.01	0.00	0.04	50.30	0.01	0.14	58.00
8.28	2.72	1.00	0.00	0.04	1.00	0.01	0.15	57.90
8.18	2.69	0.45	0.00	0.03	1.00	0.01	0.15	57.80
8.09	2.66	0.00	0.00	0.03	1.00	0.01	0.16	57.70
8.01	2.62	-0.01	0.00	0.03	1.00	0.01	0.16	57.60
6.41	2.10	1.00	0.00	0.03	1.00	0.00	0.17	55.80
5.34	1.78	0.45	0.00	0.02	1.00	0.00	0.17	54.10
4.45	1.48	0.00	0.00	0.02	1.00	0.00	0.17	52.40
3.57	1.22	-0.01	0.00	0.02	1.00	0.00	0.17	50.70
3.08	0.93	1.00	0.00	0.01	1.00	0.00	0.18	49.00
2.61	0.79	0.45	0.00	0.01	1.00	0.00	0.19	47.30
2.27	0.70	0.00	0.00	0.01	1.00	0.00	0.21	45.70
2.00	0.62	-0.01	0.00	0.01	1.00	0.00	0.22	44.20
0.02	-0.01	0.00	0.00	0.00	60.40	0.00	0.22	18.90

4. REFERENCES

CRWMS M&O 2000k. *Abstraction of Near Field Environment Drift Thermodynamic Environment and Percolation Flux.* ANL-EBS-HS-000003 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0039.

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